APPENDIX A.--METHOD OF CALCULATING RESULTS

As indicated in the text, the data from operations with both gasifiers were represented by empirical equations. (Equations for data from the water-cooled gasifier were given in an earlier Bureau of Mines publication.[10] The combined results from both sets of data were fitted by general second order equations of the form:

$$Y = b_0 + b_1 x_1 + b_2 x_2 + b_3 x_3 + b_4 x_4 + b_{11} x_1^2 + b_{22} x_2^2 + b_{33} x_3^2$$
$$+ b_{44} x_4^2 + b_{12} x_1 x_2 + b_{13} x_1 x_3 + b_{14} x_1 x_4 + b_{23} x_2 x_3 + b_{24} x_2 x_4 +$$
$$b_{34} x_3 x_4 + b_5 x_5 + b_{55} x_5^2 + b_{15} x_1 x_5 + b_{25} x_2 x_5 + b_{35} x_3 x_5 + b_{45} x_4 x_5 , \qquad (6)$$

where Y is the dependent variable, the x's with the subscripts are the independent variables, and the b's with the subscripts are the coefficients (table A-1 gives definitions of the variables).

TABLE A-1. - Coding equations for variables

Designations and units for uncoded variables:	Coding equation
Independent variables	
P = Gasifier pressure, p.s.i.g...................	$X_1 = (P - 225)/75$
C.R. = Coal rate, lb./hr.........................	$X_2 = (C.R. - 1,150)/350$
O/C = Oxygen-to-coal ratio, std. c.f./lb.........	$X_3 = (O/C - 9.82)/1.13$
s/c = Steam-to-coal ratio, lb./lb................	$X_4 = (s/c - 0.45)/.15$
H.L. = Heat loss, B.t.u./lb. of coal.............	$X_5 = (H.L. - 800)/500$
Dependent variables	
% C = Carbon gasified, percent...................	$Y_1 = (\% C - 90)/10$
C Req. = Coal requirement, lb./m. std. c.f. $CO + H_2$....................................	$Y_2 = (C Req. - 41.3)/4$
O Req. = Oxygen requirement, std. c.f./m. std. c.f. $CO + H_2$................................	$Y_3 = (O Req. - 410)/50$
H.L. = Heat loss, B.t.u./lb. of coal.............	$Y_4 = (H.L. - 800)/500$
E.G.T. = Exit-gas temperature, °F................	$Y_5 = (E.G.T. - 2,600)/457.5$

The independent variables used in correlating the second set of data were pressure, coal rate, oxygen-to-coal ratio, and steam-to-coal ratio. In correlating the combined data, the heat loss variable was added. Because the volume of the reaction zone of the refractory-lined gasifier, 3 cu. ft., was 1.5 times that of the water-cooled gasifier, coal-feed rates were given as

[10] Work cited in footnote 8, p. 10.

weight-rate per unit of reaction space. In other words, the effective coal-feed rate for the water-cooled gasifier was taken as 1.5 times the actual rate. Tests with the water-cooled gasifier included four pressure levels. Only the 150 and 300 p.s.i.g. tests were included in the correlation described in this report, however, because the tests with the refractory-lined unit were conducted only at these pressures.

A standard multiple regression procedure was used for the calculations.[11] The data were first coded by the equations in table A-1 to give a conformable matrix. The matrix was inverted, and coefficients of the coded variables were obtained. Tables A-2 and A-3, respectively, give the coefficients and their standard deviations for the second and combined sets. Except for those involving exit-gas temperature, the graphs in this report were obtained from the coefficients of table A-3. Analysis of variance is given in table A-4.

TABLE A-2. - Coefficients and their standard deviations for runs with the refractory-lined gasifiers, 92 to 104

	Carbon gasified		Coal requirement		Oxygen requirement		Heat loss		Exit-gas temperature	
	Coefficient	Standard deviation	Coefficient	Standard deviation	Coefficient	Standard deviation	Coefficient	Standard deviation	Coefficient	Standard deviation
b_0	0.237	0.0824	-1.339	0.0958	-1.136	0.0706	-0.632	0.0342	0.153	0.1005
b_1	.006	.0542	- .071	.0631	- .057	.0465	.36	.0225	-.220	.0662
b_2	.050	.0552	- .084	.0642	- .064	.0473	- .244	.0229	.129	.0674
b_3	.609	.0629	- .463	.0731	.488	.0539	.217	.0261	.408	.0767
b_{11}	.056	.0545	- .055	.0633	- .034	.0467	- .008	.0226	-.004	.0665
b_{22}	-.129	.0788	.322	.0916	.239	.0676	.125	.0327	-.087	.0962
b_{33}	-.237	.0776	.320	.0903	.198	.0666	.047	.0322	-.140	.0948
b_{12}	.078	.0804	- .068	.0936	- .038	.0690	- .011	.0334	.008	.0982
b_{13}	.116	.0587	- .088	.0683	- .087	.0504	.014	.0244	.038	.0717
b_{23}	.010	.0622	- .023	.0724	- .031	.0533	- .052	.0258	.030	.0759
b_4	-.067	.0610	.070	.0710	.057	.0523	- .033	.0253	-.207	.0745
b_{44}	-.044	.0743	- .068	.0865	- .045	.0637	- .001	.0309	-.052	.0907
b_{14}	.169	.0585	- .164	.0680	- .114	.0501	- .003	.0243	.040	.0714
b_{24}	.166	.0586	.152	.0682	.133	.0503	.009	.0243	-.056	.0716
b_{34}	.019	.0614	- .052	.0713	- .052	.0526	- .039	.0255	-.010	.0749

The equation for the data obtained from studies involving the refractory-lined gasifier included only the first 15 terms of the equation shown above. How well the curves represent the data is shown by table 11, which lists the deviations of the calculated values from the experimental values.

As in the previous work,[12] variabilities inherent in operating the gasifier, such as thickness and composition of slag on the wall and deflection of the flame by slag on the lip of the burner also apply to the tests reported here. Some of the numerical values of error have changed, however, as given under errors of measurement and standard deviations of the relations.

[11] Davies, Owen L., The Design and Analysis of Industrial Experiments: Hafner Publishing Co., 1954, New York, N.Y., pp. 552-561.

[12] Work cited in footnote 8, p. 10.

TABLE A-3. - Coefficients and their standard deviations for combined results, runs 39 to 68 and 92 to 104

	Coal requirement		Oxygen requirement		Carbon gasified	
	Coefficient	Standard deviation	Coefficient	Standard deviation	Coefficient	Standard deviation
b_0	-0.419	0.196	-0.457	0.150	-0.371	0.171
b_1	-.297	.066	-.203	.051	.226	.058
b_2	.475	.107	.376	.082	-.222	.094
b_3	-1.125	.143	.015	.110	.965	.125
b_{11}	-.040	.084	-.025	.064	.019	.073
b_{22}	.163	.044	.129	.034	-.070	.039
b_{33}	.399	.095	.265	.072	-.189	.083
b_{12}	-.243	.053	-.170	.040	.144	.046
b_{13}	.060	.068	.018	.052	-.085	.059
b_{23}	-.265	.091	-.194	.070	.080	.079
b_4	.099	.185	.066	.142	-.048	.160
b_{44}	-.087	.079	-.058	.061	-.029	.069
b_{14}	-.091	.062	-.049	.047	.081	.054
b_{24}	.079	.093	.071	.071	-.029	.081
b_{34}	-.024	.091	-.022	.070	-.013	.079
b_5	1.766	.416	1.345	.319	-1.035	.360
b_{15}	-.297	.143	-.163	.110	.366	.125
b_{25}	.597	.209	.482	.160	-.166	.183
b_{35}	-.914	.339	-.644	.259	.370	.295
b_{45}	-.056	.353	-.066	.270	.026	.308
b_{55}	.724	.395	.578	.306	-.270	.345

TABLE A-4. - Analysis of variance

Runs	Coal requirement	Oxygen requirement	Carbon gasified
39 to 68:			
Sum of squares about mean....................	29.97	42.69	25.21
Reduction due to regression..................	17.56	34.64	20.18
Residual sum of squares......................	12.41	8.05	5.03
Error mean square............................	.226	.146	.092
Standard deviation, uncoded..................	[1]1.9	[2]19	[3]3.0
92 to 104:			
Sum of squares about mean....................	29.59	15.263	29.07
Reduction due to regression..................	21.59	10.916	23.16
Residual sum of squares......................	8.00	4.347	5.91
Error mean square............................	.16	.087	.118
Standard deviation, uncoded..................	[1]1.6	[2]15	[3]3.4
39 to 68 combined with 92 to 104:			
Sum of squares about mean....................	68.30	75.04	57.81
Reduction due to regression..................	53.12	66.13	46.20
Residual sum of squares......................	15.18	8.91	11.61
Error mean square............................	.143	.084	.109
Standard deviation, uncoded..................	[1]1.5	[2]14.5	[3]3.3

[1] Lb./M std. c.f.
[2] Std. c.f./M std. c.f.
[3] Percent.

TABLE A-5. - Difference between measured and calculated values of the material requirements

Run and period	Values of independent variables			Values of deviations of requirements per M std. c.f. CO + H_2	
	Gasifier pressure, p.s.i.g.	Coal rate, lb./hr.	O_2-to-coal ratio, std. c.f./lb.	Oxygen, std. c.f.	Coal, lb.
58G	156	401	8.67	13	1.6
57B	154	409	8.53	10	1.4
57C	153	409	9.44	8	.8
57E	153	401	9.65	6	.4
58F	156	401	10.42	-9	-1.2
57D	153	409	10.22	-1	-.2
61C	155	705	8.92	0	-2.0
59P	150	703	8.95	-20	-2.2
59L	154	684	9.17	-15	-1.7
59M	154	684	10.16	-19	-2.2
59O	150	703	9.93	-10	-1.1
61D	156	705	9.94	0	.1
61E	155	705	10.70	-30	-.2
59Q	151	703	10.78	-20	-2.2
59N	154	684	10.96	-10	-1.1
65A	155	1,085	8.44	-15	-1.3
$65A_r$	155	1,087	8.43	2	.5
62F	157	1,019	9.00	12	2.1
63J	155	986	9.24	35	3.8
62J	158	981	9.28	15	1.5
65B	155	1,085	9.34	0	.1
$65B_r$	151.5	1,087	9.31	9	.9
66A	156	971	9.43	1	0
60T	155	931	9.80	10	.9
62I	158	981	10.30	9	-.7
63I	151	986	10.35	17	1.5
66B	156	971	10.45	0	0
62G	159	1,019	10.71	0	-.3
60U	156	931	10.91	21	1.8
68K	299	415	8.37	-5	.2
67F	300	396	8.81	-51	-5.6
68J	300	415	9.28	0	0
67G	300	396	9.87	7	.6
68I	300	415	10.08	-2	-.2
67I	298	402	10.52	25	2.4
47E	300	730	8.29	-8	-.6
44K	300	692	8.66	-9	-.7
47G	300	730	8.92	-14	-1.1
47F	300	730	9.72	-6	-.4
43E	300	647	10.15	-23	-1.9
66E	300	745	10.22	49	39
40C	300	831	10.88	0	0
43D	300	647	10.89	-6	-.5
$66E_r$	295	675	11.32	-7	-.6
40B	300	831	11.38	-8	-.6
40A	300	831	13.03	-2	-.1
47D	300	1,062	8.81	0	0
42C	300	1,002	9.37	11	.8
44J	300	1,054	9.63	5	.4
42B	300	1,002	10.17	6	.5
47C	300	1,062	10.40	-3	-.3
44I	300	1,054	10.50	8	.6
42A	300	1,002	10.92	-7	-.5
39B	300	1,200	12.29	-4	-.4
39C	300	1,108	12.85	11	.9
39A	300	1,200	12.90	-1	-.1
43F	300	1,437	8.95	-5	-.4
48B	300	1,341	9.49	-9	-.7
44G	300	1,437	9.63	-9	-.7
48F	300	1,341	10.28	-30	-2.4
44H	300	1,437	10.41	18	1.5
48E	300	1,341	11.17	-13	-1.0

Run and period	Values of independent variables				Values of deviations of requirements per M std. c.f. CO + H_2	
	Gasifier pressure, p.s.i.g.	Coal rate, lb./hr.	O_2-to-coal ratio, std. c.f./lb.	Steam-to-coal ratio, lb./lb.	Oxygen, std. c.f.	Coal, lb.
100D	150	772	8.78	0.31	-2	0
94E	150	817	8.23	.29	-4	-0.3
92C	150	806	8.33	.61	-20	-2.3
101B	150	800	8.49	.60	34	1.5
102E	150	778	10.87	.31	6	.8
93D	150	796	10.47	.30	2	.4
95B	150	798	10.51	.61	-1	-.2
99C	150	750	11.20	.64	21	1.8
93E	150	1,485	8.55	.32	-15	-1.7
102A	150	1,475	8.61	.30	0	-.1
95E	150	1,498	8.54	.60	4	.8
100E	150	1,538	8.34	.58	-19	-1.8
99E	150	1,522	10.23	.30	-2	-.1
94A	150	1,495	10.64	.32	-2	0
92A	150	1,484	10.65	.61	14	1.2
101D	150	1,484	10.62	.60	-9	-2.1
92E	225	1,179	9.30	.46	1	0
93C	225	1,164	9.27	.46	-2	-.3
94B	225	1,155	9.68	.46	-9	-1.1
95A	225	1,093	10.00	.48	-3	-.4
96D	225	1,176	9.33	.44	10	1.0
97C	227	1,155	9.49	.44	-2	-.4
98B	225	1,122	9.72	.46	0	-.1
99D	225	1,140	9.76	.45	-3	-.3
100B	225	1,173	9.36	.45	-10	-1.1
101C	225	1,153	9.53	.44	-22	-2.3
102B	225	1,097	9.86	.47	-12	-1.3
103A	225	1,054	8.78	.49	6	.8
103E	225	1,171	9.16	.44	-13	-1.5
104A	225	1,105	9.77	.47	2	.1
95C	300	787	8.61	.30	4	.4
$101E_r$	300	805	8.35	.30	11	1.5
100C	300	785	8.55	.61	6	1.1
93A	300	797	8.48	.62	-18	-1.8
92D	300	834	9.92	.29	26	2.5
98A	300	835	10.08	.29	-7	-.8
100T	300	814	10.29	.30	19	1.7
99B	300	756	10.87	.32	-7	-.8
101A	300	784	10.81	.61	-15	-1.5
94D	300	812	10.38	.59	-16	-1.5
100A	300	1,457	8.84	.30	-6	-1.0
92B	300	1,593	8.10	.30	10	1.7
94C	300	1,509	8.46	.60	14	-.1
102D	300	1,456	8.70	.62	14	1.9
102C	300	1,445	10.83	.31	4	.4
95D	300	1,476	10.64	.31	13	1.3
$93B_r$	300	1,484	10.78	.61	6	1.8
99A	300	1,432	11.10	.62	-13	.3
93B	300	1,623	9.57	.55	-6	-.4
97B	119	1,142	9.57	.45	0	.1
104E	119	1,098	9.83	.47	1	.4
103D	330	1,145	9.59	.44	1	-.1
97D	330	1,156	9.40	.45	12	1.1
96A	225	696	8.93	.42	43	4.7
103B	225	658	9.39	.45	16	1.5
96C	225	1,646	9.48	.44	-1	.1
103C	225	1,649	9.47	.45	2	.1
103A	225	1,146	8.16	.44	2	.4
97E	225	1,111	8.35	.47	3	.8
97A	225	1,121	11.24	.46	3	.2
104D	225	1,141	10.96	.46	-3	-1.1
104C	225	1,114	9.69	.25	-1	-.1
96E	225	1,150	9.52	.24	4	.3
96B	225	1,125	9.73	.67	8	.8
104B	225	1,099	9.81	.61	-6	-.5

APPENDIX B.--DETERMINATION OF FRACTION OF HEAT LOSS EQUIVALENT TO $CO + H_2$

The fraction of heat loss converted to $CO + H_2$ is the rate of decrease of the latter with increasing heat loss multiplied by the reaction heat required to produce a unit of $CO + H_2$. The coal requirement is the reciprocal of standard cubic feet of $CO + H_2$ per pound of coal, and the heat loss is expressed in terms of pounds of coal. Then

$$f = - \frac{d(1/C_r)}{d\ HL} (H) = \frac{H}{C_r^2} \frac{dC_r}{dHL}, \qquad (7)$$

where

f = fraction of heat loss converted to $CO + H_2$,

C_r = coal requirement, lb./M std. c.f. $CO + H_2$,

HL = heat loss, B.t.u./lb. of coal,

and H = heat of reaction, B.t.u./M std. c.f. $CO + H_2$.

The ratio $\frac{dC_r}{dHL}$ is found from the coal requirement correlation.

APPENDIX C.--DERIVATION OF SLOPES OF CURVES SHOWING CHANGE IN COAL AND OXYGEN REQUIREMENTS WITH CHANGE IN HEAT LOSS

The mathematical expressions for the change of coal and oxygen requirements with change in heat loss are given by the equations:

$$\frac{dC_r}{dHL} = \frac{4}{500} \frac{dy_2}{dx_5}, \tag{8}$$

and

$$\frac{dO_2}{dHL} = \frac{50}{500} \frac{dy_3}{dx_5}. \tag{9}$$

These equations are changed to a usable form by differentiating with respect to heat loss. For example, for coal requirement, this gives

$$\frac{dy_2}{dx_5} = b_5 + b_{15}x_1 + b_{25}x_2 + b_{35}x_3 + 2b_{55}x_5. \tag{10}$$

The oxygen requirement is handled similarly. Substituting the values of the coefficients from table A-3, the values of the slopes for the coal and oxygen requirement equation given on page 15 are obtained.

APPENDIX D.--MATHEMATICAL DERIVATION OF VALUES FOR OPTIMUM CAPACITY OF THE GASIFIER

As discussed in the text, the optimum gasifier capacity is that which gives the lowest material requirements (coal and oxygen) per unit of $CO + H_2$ produced.

The optimum capacity is derived as follows:

$$\frac{dC_r}{dR} + a\frac{dO_r}{dR} = -\left[\frac{dC_r}{dHL} + a\frac{dO_r}{dHL}\right]\frac{(dHL)}{dR} \qquad (11)$$

where

a is the relative cost of oxygen and coal--the cost of 1 std. c.f. of O_2 divided by the cost of 1 lb. of coal.

Assuming a is equal to 0.1, conversion to coded variables gives

$$\frac{4}{350}\frac{dy_2}{dx_2} + (0.1)\frac{50}{350}\frac{dy_3}{dx_2} = \left[\frac{4}{500}\frac{dy_2}{dx_5} + (0.1)\frac{50}{500}\frac{dy_3}{dx_5}\right]\left[-\frac{500}{350}\frac{dy_4}{dx_2},\right]$$

or

$$\frac{dy_2}{dx_2} + 1.25\frac{dy_3}{dx_2} = \left[\frac{dy_2}{dx_5} + 1.25\frac{dy_3}{dx_5}\right]\left[-\frac{dy_4}{dx_2}\right]$$

(Note: y_4 and x_5 are two different ways of expressing heat loss in B.t.u./lb. of coal; y_4 is determined from a correlation equation; x_5 is an experimental value or an assumed value.)

From table A-3

$$\frac{dy_2}{dx_2} + 1.25\frac{dy_3}{dx_2} = 0.945 - 0.456x_1 + 0.648x_2 - 0.507x_3 + 0.168x_4 + 1.20x_5;$$

$$\frac{dy_2}{dx_5} + 1.25\frac{dy_3}{dx_5} = 3.45 - 0.50x_1 + 1.20x_2 - 1.72x_3 - 0.14x_4 + 2.89x_5.$$

From table A-2

$$\frac{dy_4}{dx_2} = 0.244 + 0.011x_1 - 0.250x_2 + 0.052x_3 - 0.009x_4.$$

Because x_4 has a negligible effect, it was assumed to be zero.

Then

$$\begin{aligned}&0.945 - 0.456x_1 + 0.648x_2 - 0.507x_3 + 1.20x_5\\&= (3.45 - 0.50x_1 + 1.20x_2 - 1.72x_3 + 2.89x_5)(0.244 + 0.011x_1\\&\qquad - 0.250x_2 + 0.052x_3)\end{aligned} \qquad (12)$$

Taking values for x_1 and x_3, this equation can be solved simultaneously with the correlation equation for the heat loss to give values for x_2, the coal-feed rate, which is the desired value.

APPENDIX E.--CALCULATION OF EXIT-GAS TEMPERATURES

Definition of Terms

Energy balance basis: 1 pound of coal

c	= carbon, moles/lb. of coal
w	= moisture + combined water, moles/lb. of coal
h	= net H_2, moles/lb. of coal
f	= fraction of carbon gasified
u	= process oxygen, std. c.f./lb. of coal
s	= process steam, lb./lb. of coal
d	= CH_4 produced, moles/lb. of coal
e	= unsaturated hydrocarbons (assumed C_2H_4) produced, moles/lb. of coal
HV	= gross heating value of coal, B.t.u./lb.
C_{pw}	= molal specific heat of steam, B.t.u./lb. - mole/° F.
C_{pO2}	= molal specific heat of oxygen, B.t.u./lb. - mole/° F.
C_{px}	= molal specific heat of x constituent of product gas, B.t.u./lb. - mole/° F.
A	= ash content of coal, lb./lb.
C_{pash}	= specific heat of ash, B.t.u./lb./° F.
HL	= heat loss from gasification section, B.t.u./lb. of coal
x	= CO_2 produced, moles/lb. of coal
HV_x	= gross heating value of x gaseous constituent, B.t.u./lb. - mole
T_{in}	= temperature of steam and oxygen entering, ° F.
T_o	= base temperature, ° F.
T	= temperature of gas leaving reaction zone, ° F.
C_{pc}	= specific heat of ungasified carbon, B.t.u./lb./° F.
P	= undecomposed steam leaving gasifier, lb./lb. of coal
k	= water-gas shift equilibrium constant

Average Values for Conditions of Runs

C_{pw}	= 0.4556	c	= 0.0590
C_{pO2}	= 0.01905	h	= 0.0211
T_{in}	= 500° F.	w	= 0.0044
T_o	= 80° F.	d	= 0.0005
C_{pash}	= 0.326	e	= 0.0005
C_{pgas}	= 7.38 + 0.00045 T	Ash	= 0.138
C_{pc}	= 0.252 + 0.00013 T		

Heating Values

Coal (c)	12,765 B.t.u./lb.
CH_4 (d)	382,540 B.t.u./mole
C_2H_4 (e)	620,300 B.t.u./mole
$CO + H_2$	122,540 B.t.u./mole
Ungasified carbon	173,940 B.t.u./mole of carbon

Heat of fusion of ash = 25 B.t.u./lb. of coal

Material Balance Equations

If reactions are

$$dC + 2d\,H_2 \rightarrow dCH_4 ,$$

$$2eC + 2e\,H_2 \rightarrow eC_2H_4 ,$$

$$(cf-d-2e)C + (s/18 + W)H_2O \rightarrow (cf-d-2e)\,(CO + H_2) + (s/18 + w-cf + d + 2e)H_2O,$$

and $$(h+cf-3d-4e)H_2 + 1/2(u/189)O_2 \rightarrow (h-cf-3d-4e-u/189)H_2 + (u/189)H_2O$$

$$xCO + xH_2O \rightarrow xCO_2 + xH_2 .$$

Moles leaving:

$$CH_4 = d,$$
$$C_2H_4 = e,$$
$$H_2 = h + cf - 3d - 4e - u/189 + x,$$
$$CO = cf - d - 2e - x,$$
$$H_2O = s/18 + w + u/189 + d + 2e - cf - x,$$
$$CO_2 = x,$$

and $$\text{Total} = -2d - 3e + h + cf + s/18 + w.$$

In the term for specific heat of the gas, d + e has been added to the above total to allow for the increased specific heat of CH_4 and C_2H_4.

Heat Balance

Gross heat of combustion of coal + sensible heat of entering steam and oxygen + latent heat of entering steam = gross heat of combustion of CO and H_2 + sensible heat of product gases + latent heat of undecomposed steam + sensible heat of ash + sensible heat of ungasified carbon + heat of fusion of ash + heat loss from reaction zone + heat of combustion of ungasified carbon + gross heat of combustion of CH_4 and C_2H_4.

$$HV + \left(\frac{s}{18} Cpw + \frac{u}{378} C_pO_2\right)(T_{in} - T_o) + 173{,}940\ c(1 - f)$$

$$+ HV_{CH_4}\ d + HV\ C_2H_4\ e + HV_{H_2}\ \left(h + cf - dc - 4e - \frac{u}{189} + x\right)$$

$$+ HV_{CO}\ (cf - d - 2e - x) + (T - T_o)\ AC_p ash$$

$$+ (T - T_o)\ 0.708\ (1 - f)\ (0.252 + 0.00013T)$$

$$+ (T - T_o)\ (C_p gas\ avg.)\ \left(-d - 2e + h + cf + \frac{s}{18} + w\right) + HL + 25\ (T - T_o)$$

$$= HV + \left(\frac{s}{18} C_{pw} + \frac{u}{378} C_pO_2\right)(T_{in} - T_o) - \Big[173{,}940\ c(1-f)$$

$$+ HV_{CH_4} d + HV_{C_2H_4} e + HV_{H_2}\ \left(h + cf - 3d - 4e - \frac{u}{189} + x\right)$$

$$+ HV_{CO}\ (cf - d - 2e - x)\Big] + 25 - HL \Big/ \Big[A\ C_p ash + C_p gas\ avg.$$

$$\left(-d - 2e + h + cf + \frac{s}{18} + w\right) + 0.708\ (1 - f)\Big]$$

After substitution of the foregoing given values and algebraic manipulation, the following equation results

$$\frac{T^2}{100}\ (1.028 + 0.25s - 0.6545f) + \frac{T}{100}\ (39.23 + 40.8s + 26.2f)$$

$$= 661u + 1{,}284s - 19{,}080P - 4{,}286f - HL + 66.$$

This may be solved by the quadratic formula after determination of the value of P as described in the next section.

Substituting values from the material balance equations:

$$(1 - k)P^2 - \Big[h + w\,(2 - k) + \frac{s}{18}\,(2 - k)$$

$$+ (1 - k)\,\frac{u}{189} - d\,(1 + 2k) - 4ek - cf\,(1 - 2k)\Big]\,P$$

$$+ \left(w + \frac{s}{18} + \frac{u}{189} + d + 2e - cf\right)\left(w + \frac{s}{18} - 2d - 2e + h\right) = 0$$

If we assume k to be a constant corresponding to the average equilibrium constant found for the actual experiments, then the above equation can be solved for P. The value of k used was 0.435, which corresponds to an equilibrium temperature of 2,100° F.

Determination of P

Assume water-gas shift reaction is at equilibrium:

$$k = \frac{(CO_2)(H_2)}{(CO)(H_2O)}\ .$$

Let $H_2 + H_2O = C$,

$CO + H_2 = A$,

and $CO_2 + H_2O = B$;

then $H_2 = C - H_2O$,

$CO_2 = B - H_2O$,

and $CO = A - C + H_2O$

$$k = \frac{(B - H_2O)(C - H_2O)}{(A - C + H_2O)\ H_2O}\ .$$

$$(H_2O)^2\,k + (A - C)\,k\,H_2O - BC - H_2O^2 + H_2O\,(C + B) = 0,$$

$$(H_2O)^2\,(k - 1) + \Big[k(A - C) + C + B\Big]\,H_2O - BC = 0,$$

or $$H_2O^2\,(1 - k) - H_2O\Big[k(A - C) + C + B\Big] + BC = 0,$$

and $H_2O = P$.