B.I.O.S. MISCELLANEOUS REPORT No. 39.

GRAPHICAL REPRESENTATIONS OF GAS PRODUCER PROCESSES

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Graphical Representations of Gas Producer Processes

Since Gibb's application of triangular coordinates for the representation of chemical compositions, graphical representations were used generally in all fields of chemistry.

One of the most comprehensive publications on the graphic representations of combustion processes of carbon and hydrocarbons is W. Ostwald's "Contribution to the Graphic Combustion Technique" (in German) Edition Spamer, Leipzig, 1920.

Ostwald's triaxal representation of the carbon dioxide, oxygen and carbon monoxide content of flue gases of engines and furnaces and Ackermann's triangle considering these gases in combination with unburned carbon (soot) in diesel engine flue gases seem to be known to all engineers.

The conditions encountered in gas producer processes were shown graphically by Ostwald in the above mentioned book using triangular coordinates. The corners of the equilateral triangle correspond to the three equations.

point A $C + O_2 = CO_2$

" B $C + 2 H_2O = CO_2 + 2 H_2$

" C $C + CO_2 = 2 CO$

A small equilateral triangle with point C and with an area of one fourth of the triangle ABC is unused because conditions in it require the addition of carbon dioxide to carbon instead of oxygen. Omitting this small triangle an isosceles trapezium remains, which gave the idea to use a quadrilateral one in order to represent the carbon gasifying reactions.

It shall be premised that all these graphical representations have theoretical significance only. They are helpful in order to become familiar with the theory and to interpret gas properties and performed gas analyses, so that they present an important auxiliary means. The graphs have the drawback in common with all other stoichiometric representations in that, they do not offer a deeper insight in the processes than is already inherent in the chemical equations. Furthermore, the graphs require more or less simplifying assumptions, so that representations of the gasification of bituminous coals for example with its secondary reactions, become inexact.

However, we find in literature various enlargements of application and derivations of the original Ostwald triangle and a somewhat spread application in the practice of gas producing, so that it seems reasonable to represent the development of a gasification trapezoid, used successfully in my former laboratory (at the Institute of Technology of Fuels at the Technical University of Vienna) and unpublished until now.

The four reactions of carbon with air and water steam, which determine all possible gasification operations and which present the four angles of the gasification rectangle according to figure 1, are:

A Combustion with air (gasification to CO_2)

$$C + O_2 + 3.76\ N_2 = CO_2 + 3.76\ N_2 + 97{,}000 \text{ calories}$$

B Combustion with water (gasification to CO_2 and H_2)

$$C + 2\ H_2O = CO_2 + 2\ H_2 - 18{,}200 \text{ calories}$$

C Gasification with water to CO and H_2

$$C + H_2O = CO + H_2 - 28{,}300 \text{ calories}$$

D Gasification with air to CO

$$C + 0.5\ O_2 + 1.88\ N_2 = CO + 1.88\ N_2 + 29{,}300 \text{ calories}$$

It does not matter in our representation that, in agreement with newer gas producer theories, the reaction B does not take place practically, since it consists of two reactions which are superposed simultaneously:

$$C + H_2O = CO + H_2 - 28{,}300 \text{ calories}$$

$$CO + H_2O = CO_2 + H_2 + 10{,}100 \text{ "}$$

$$\text{Sum} \quad C + 2\,H_2O = CO_2 + 2H_2 - 18{,}200 \text{ "}$$

Coordinating the four reactions A, B, C and D, to the corners of a rectangle, we are able to represent for each point of its area:

1) the gas compositions, namely CO_2, CO, H_2 and N_2 contents in per cent by volume,

2) the gas volumes produced from the unit of carbon, as moles or cubic meters of gas per mole or kg carbon or the carbon content in kg of the unit of gas,

3) the reaction heat as a positive or negative heat evolution per unit of carbon or per unit of gas,

4) the gross and net thermal value, of the produced gases related to one mole carbon, to one normal cubic meter of gas or to one kg of carbon, the latter designated as gross or net heat value number,

5) the thermal efficiency of gasification,

6) the gas composition according to the chemical equilibria and

7) procedures occuring in gas producers.

Secondary reactions such as the formation of methane and the procedures in the presence of volatile matters, the gasification applying oxygen enriched air and the degree of water decomposition require derived graphs, but shall not be aim of contemplation of this report.

Using a square for the representation according to a proposal of W. Ostwald, the lines of gas compositions, gas volumes, reaction heats, thermal values and of the thermal efficiencies would be curves as shown partly in figure 2. The analytic - geometric equations of these curves and its design are somewhat complicated, whereas the representation by means of a trapezoid offers the advantage of straight lines for all above named values and furthermore the advantage of better imaginable representation.

It appears more logically to make (see figure 2) the side A D equal to 34.6 parts of carbon monoxide according to the 50.0% of carbon monoxide of side BC, than to have the same lengths for both of the sides AD and BC. Shortening the square side DC to (D) (C), corresponding to 50.0% H_2 of the side AB graduated in 66.7% H_2, helps improve the imagination too and corresponds better to the reaction conditions.

The design of the gasification trapezoid is shown in figures 3 and 4 and the gas analyses of the characteristic points given in table 1. The CO, H_2 and CO_2 scales are easily to apply using a millimeter or an inch graduated paper. The N_2 graduation gives no whole number graduation, on line A B, so that for a more easy scaling an auxiliary line A x - B is used in figure 4 with the aid of a line parallel to B C through A. A x - B is made 2 x 79 (% N_2) = 158 parts equal 158 millimeters.

In figure 5 the CO_2, CO, H_2 and N_2 content of the gasification trapezoid is shown stereoscopically. The gas contents form oblique wedges superposed to a prism with the congruent trapezoid A' B' C' D' at the top. Stretching out the mantle of the prism, the triangular and the trapezoid shaped side areas of the four wedges are to be seen in figure 5 above.

TABLE 1

Calculation Results of Characteristic Points

1	2	3	4	5	6	7	8	9	10	11	12	13
	1 Mole C reacting with moles of			Produced Moles of Gases				Sum of Produced Gas Moles	Gas Composition in Vol. %			
Point	O_2	N_2	H_2O	CO_2	CO	H_2	N_2		CO_2	CO	H_2	N_2
A	1.000	3.760	-	1.000	-	-	3.76	4.76	21.0	-	-	79.0
B	-	-	2.000	1.000	-	2.000	-	3.00	33.0	-	66.7	-
C	1.000	-	1.000	-	1.000	1.000	-	2.00	-	50.0	50.0	-
D	0.500	1.880	-	-	1.000	-	1.880	2.88	-	34.6	-	65.4
E	0.158	0.595	1.685	1.000	-	1.685	0.595	3.28	30.5	-	51.4	18.1
F	0.246	0.923	0.509	-	1.000	0.509	0.923	2.43	-	41.1	20.8	38.1
G	0.253	0.975	0.494	0.0124	0.987	0.494	0.975	2.47	0.5	40.0	20.0	39.5
H	-	-	1.337	0.337	0.664	1.337	-	2.34	14.4	28.4	57.2	-
P	0.423	1.603	0.399	0.250	0.750	0.399	1.603	3.00	6.3	25.0	13.3	55.4

TABLE 1 (Continued)

1	14	15	16	17	18	19	20	21
Point	Cubic meter 1 Mole C	Gas per 1 Kg C	Heat Value of Gas in Cal. per 1 Mole C	mm^3	Kg C *	Heat Evolution, Cal. per 1 Mole C	1 Kg C	Thermal Efficiency %
A	106.5	8.88	-	-	-	+ 97,000	+ 8080	-
B	67.2	5.60	115,180	1720	9600	- 18,200	- 1515	119
C	44.8	3.73	125,290	2800	10440	- 28,300	- 2360	129
D	64.5	5.37	67,700	1050	5640	+ 29,300	+ 2440	70
E	73.5	6.12	97,000	1320	8080	± 0	± 0	100
F	54.5	4.55	97,000	1780	7700	± 0	± 0	100
G	55.3	4.61	95,250	1720	7930	+ 1,750	+ 140	98
H	52.5	4.37	122,000	2320	10200	- 25,000	- 2080	126
P	67.2	5.60	74,000	1100	6150	+ 23,000	+ 1915	76

* Also: Net Gas Heat Value Number

The edges of the gas content wedges run along the lines D' - A' - B" - C - D. The dash dotted lines in figure 5 are auxiliary lines for the design of the gas composition prism and show for example, that the line D C of the trapezoid intersects at the point K with the extended CO_2 - content-line A" - B".

Figure 6 shows the readings of the gas composition of a certain point P. The N_2 scale is not necessary because the N_2 content is to be obtained by difference. In figures 7 and 8 the volumes and the heat values of the gases are represented, whereas figure 9 shows the heat evolutions, gasification efficiencies and the temperature, belonging to the gas compositions in case of complete adjustment of the Boudouard and the heterogeneous water gas equilibrium.

The construction of the graphs 7, 8 and 9 is performed using the scales on the sides of the trapezoid. These scales are calculated by means of the above four stoichiometric equations and the actual part of participation x, u, y and z of the reactions, whereby

$x \neq u = 1$, $u \neq y = 1$, $y \neq z = 1$ and $x \neq z = 1$

Some of the possible functions between gas compositions and x, u, y and z are given in table 2, whereas all values pertaining to the corners, A, B, C and D and of certain points E, F, G, H and P, are to be found in table 1. Table 3 contains the equations for heat evolution at the sides of the trapezoid as functions of the actual parts of reaction participation. Equations for gas heat values and thermal efficiency are not necessary.

Table 3 Heat Evolution Equations

A - B	$Q = 115,200\ x - 18,200$	calories
B - C	$Q = -10,100\ y - 18,200$	"
C - D	$Q = 57,600\ z - 28,300$	"
D - A	$Q = 67,700\ x \neq 29,300$	"

In figure 7 the parallel lines of gas volume values range from 8.9 m^3 in A down to 3.7 m^3 in C. The net gas heat value numbers, that means the products of net heat values of gases multiplied by the volume of gas in m^3, produced from one kg of carbon, lie on diverging straight lines. The three straight lines A - G, A - C and A - H coordinate to points with an H_2/CO ratio of 0.5, 1.0 and 2.0 respectively.

Point G represents an ideal gas, produced with 98% thermal gasification efficiency with the composition.

CO_2 = 0.5 CO = 40.0 H_2 = 20.0 N_2 = 39.5%

The lines of net and gross calorific gas values in figure 8 run parallel, whereas the lines of heat evolution and thermal efficiency in figure 9 converge to a point outside of the trapezoid. The lines of heat evolution would be congruous with those of thermal efficiency when the calorific value of one mole carbon would be 100,000 calories. They are practically congruent in the area 90% to 130% efficiency and + 10,000 to - 28,300 calories heat evolution respectively and diverge but as little as 0.5% and 5000 calories respectively in the range as far as line through D.

In figure 10 the areas are represented in which the producer gases, water gases and synthesis gases are placed. The analyses of gases drawn from the zones of a gas producer in order to investigate the procedures, represent the procedure in a coke fed gas producer. Analysis (a) relates to the combustion zone, analyses (b) to (e) to the reduction zone and (f) to the preheating zone of the producer.

The lines I, II and III show schematically the course of analyses during blow and run of water gas production and improved operation conditions, which lead from the early processes of the "European Watergas Company"

TABLE 2

Gas Composition-Formulas pertaining to the Sides of Trapezoid

Sides	Reaction equations multiplied by completion grades	Vol % of gases as functions of completion grades	Correlation between gas components
A–B	$x\,(C + O_2 + 3.76\,N_2) =$ $= x\,(CO_2 + 3.76\,N_2)$	$H_2 = \frac{1 - x}{1.5 + 0.88\,x} \cdot 100\%$ $CO_2 = \frac{1}{3 + 1.76\,x} \cdot 100\%$	$H_2 = \frac{CO_2 - 21.0}{12.3} \cdot 66.7\%$
B–C	$u\,(C + 2\,H_2O) =$ $= u\,(CO_2 + 2\,H_2)$	$CO = \frac{y}{3 - y} \cdot 100\%$ $CO_2 = \frac{1 - y}{3 - y} \cdot 100\%$	$H_2 = (50 - CO)\,\frac{16.7}{50} + 50\%$
C–D	$y\,(C + H_2O) =$ $= y\,(CO + H_2)$	$H_2 = \frac{y}{2.88 - 0.88\,y} \cdot 100\%$ $N_2 = 1.88\,z \cdot 100\%$	$H_2 = \frac{CO - 34.6}{15.4} \cdot 50\%$
D–A	$z\,(C + 0.5\,O_2 + 1.88\,N_2 =$ $= z\,(CO + 1.88\,N_2)$ $x\,(C + O_2 + 3.76\,N_2) =$ $= x\,(CO_2 + 3.76\,N_2)$	$CO = \frac{1 - x}{2.88 + 1.88\,x} \cdot 100\%$ $CO_2 = \frac{x}{2.88 + 1.88\,x} \cdot 100\%$	$CO = 34.6 - 1.65\,CO_2\%$

and the "Dellwick - Fleischer - Process" to the Strache - Water gas Process" and other modern water gas processes.

Hydrogen formation by conversion of water gas lead finally to the corner B and can be completed using low temperatures according to equilibrium temperatures shown in figure 9.

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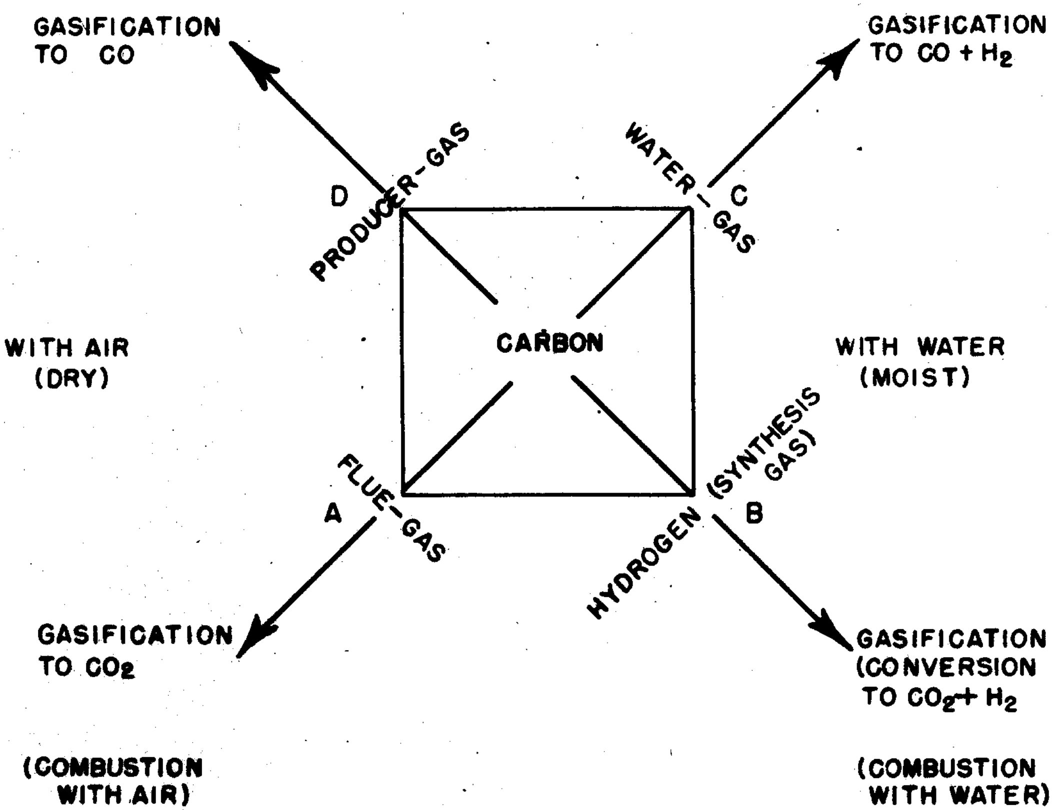

FIG. I BASIC IDEA OF A GASIFICATION RECTANGLE

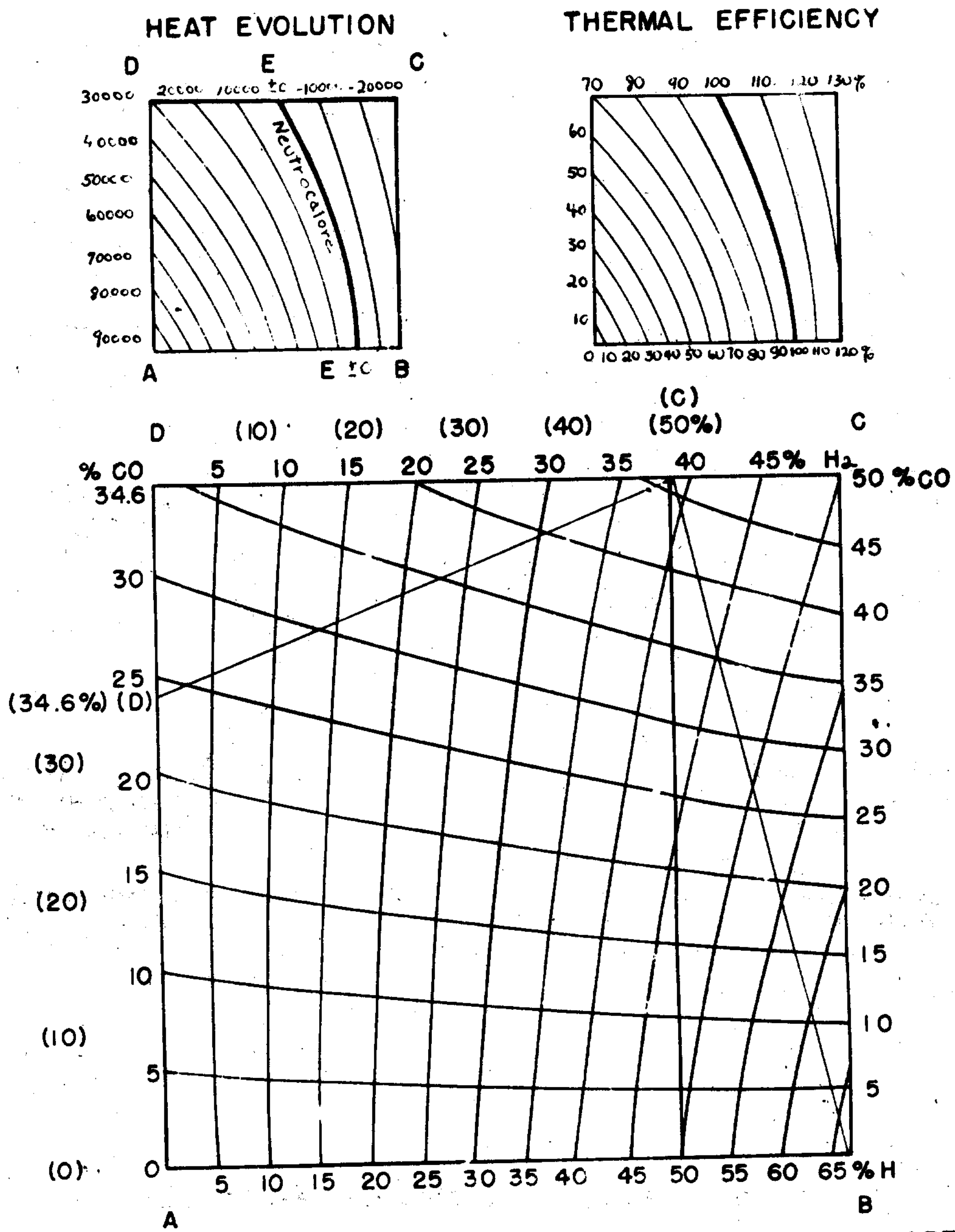

FIG 2 W. OSTWALD'S PROPOSAL OF A GASIFICATION SQUARE

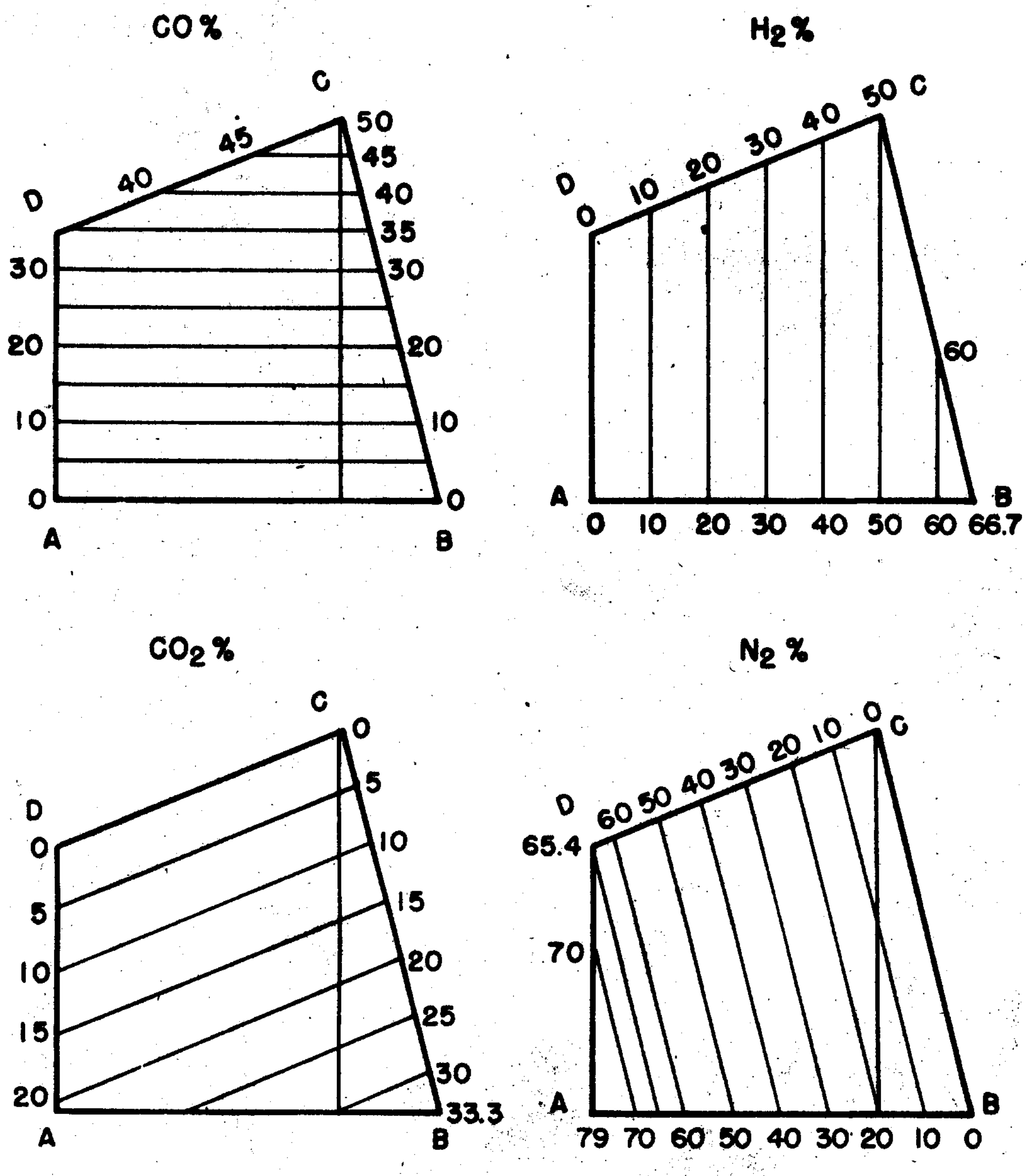

FIG. 3 SCALES OF CO, H_2, CO_2, N_2 IN GASIFICATION TRAPEZOID

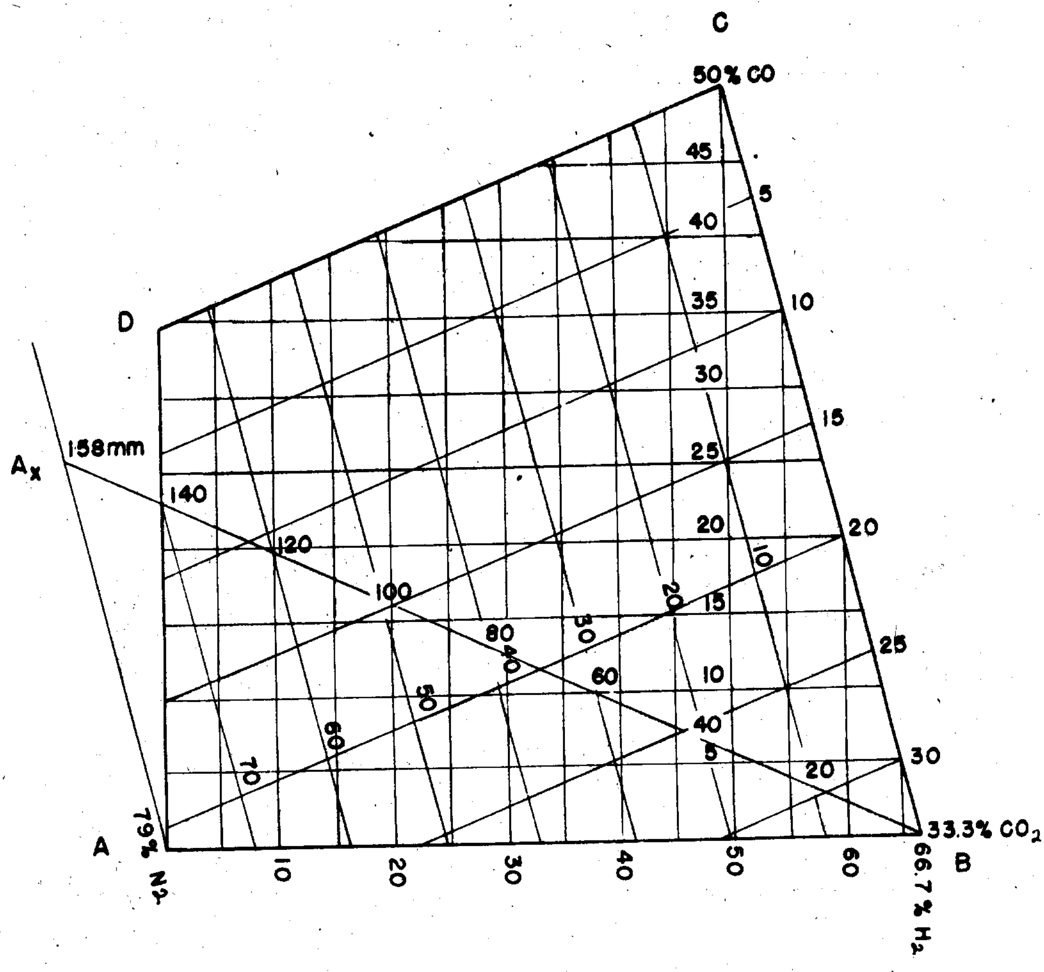

FIG. 4 DESIGN OF GASIFICATION TRAPEZOID

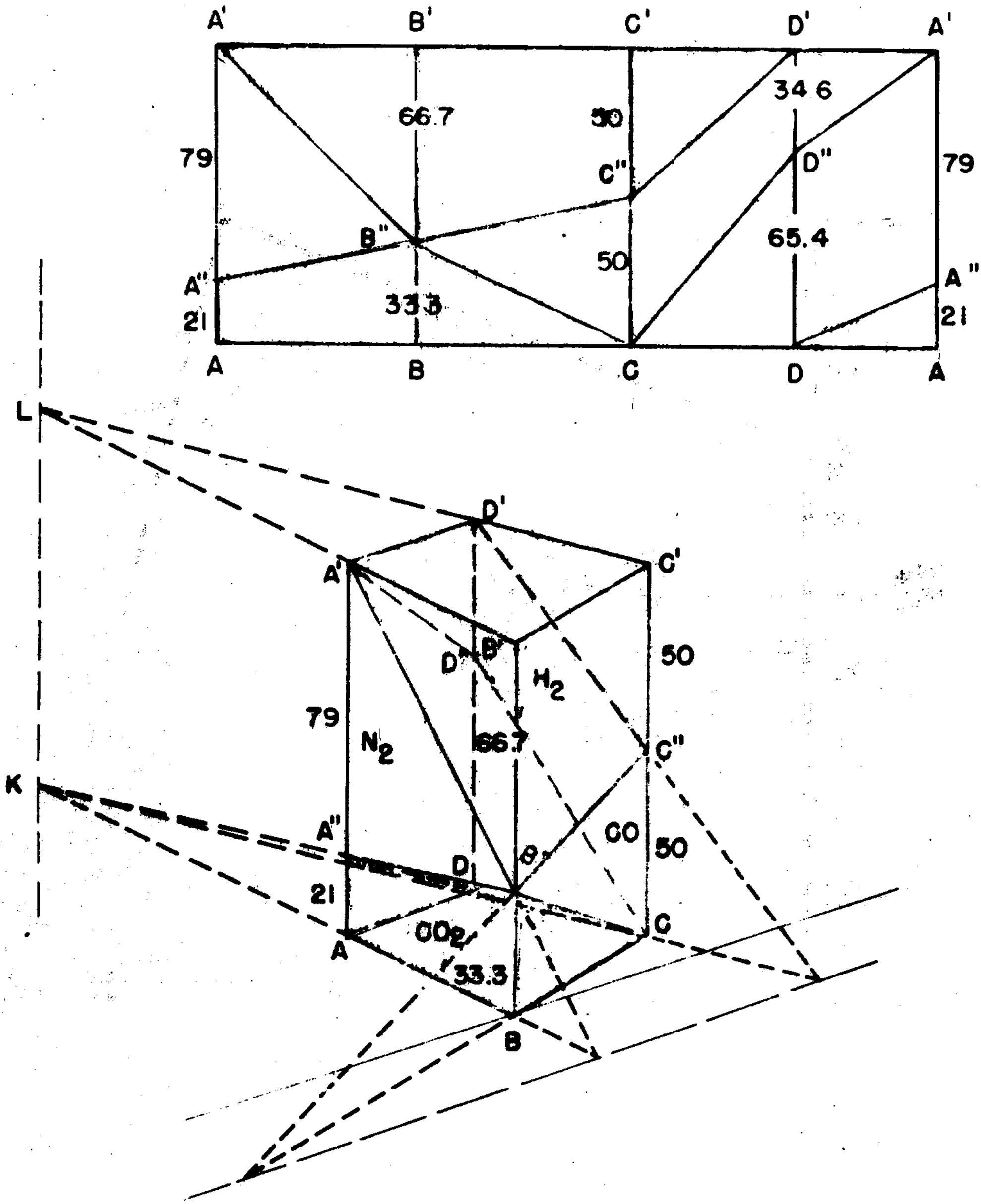

FIG. 5 STEREOSCOPIC REPRESENTATION OF GAS COMPOSITION

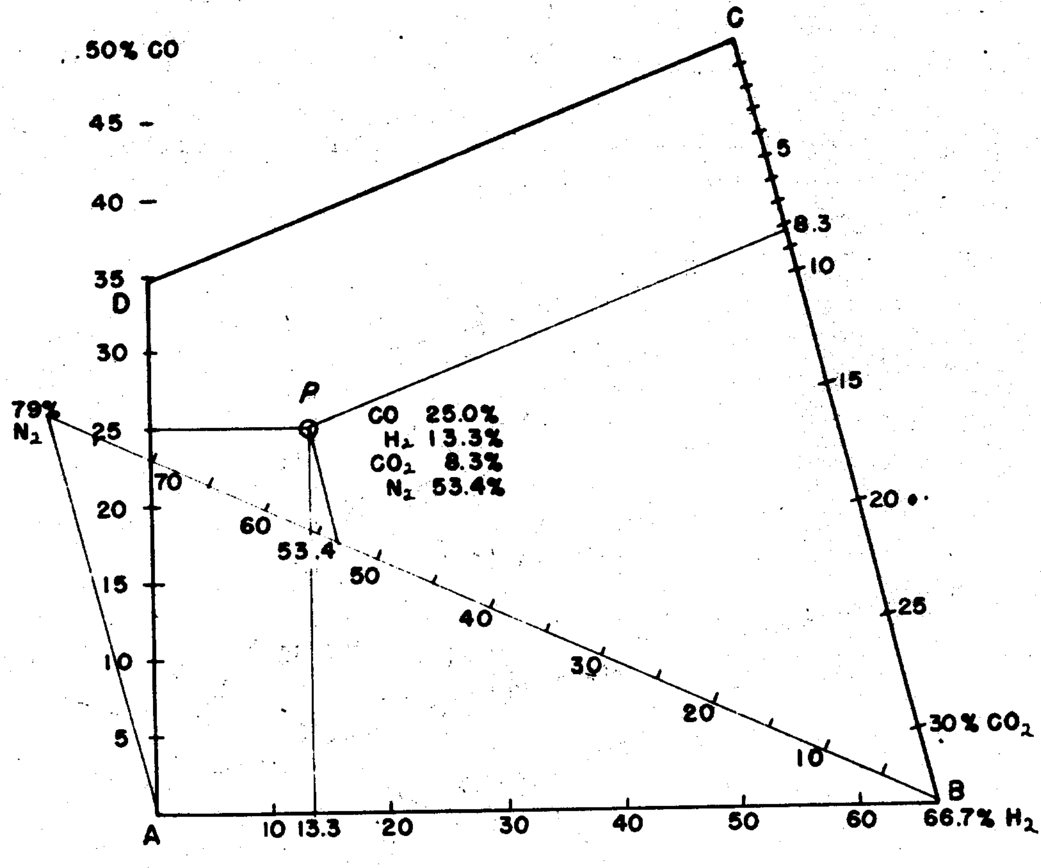

FIG. 6 READINGS OF GASCOMPOSITION OF A POINT (P)

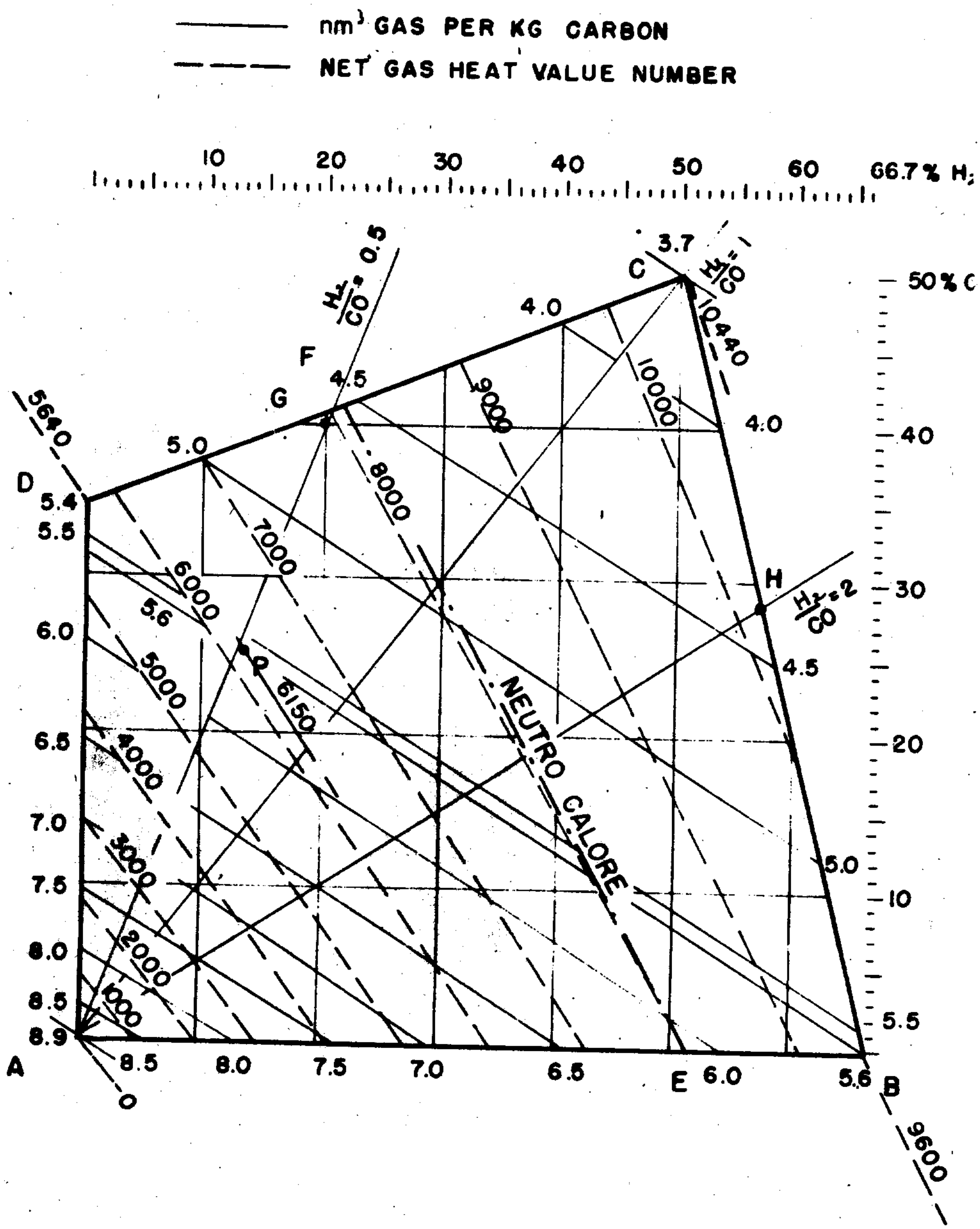

FIG 7 GAS VOLUME & NET GAS HEAT VALUE NUMBER

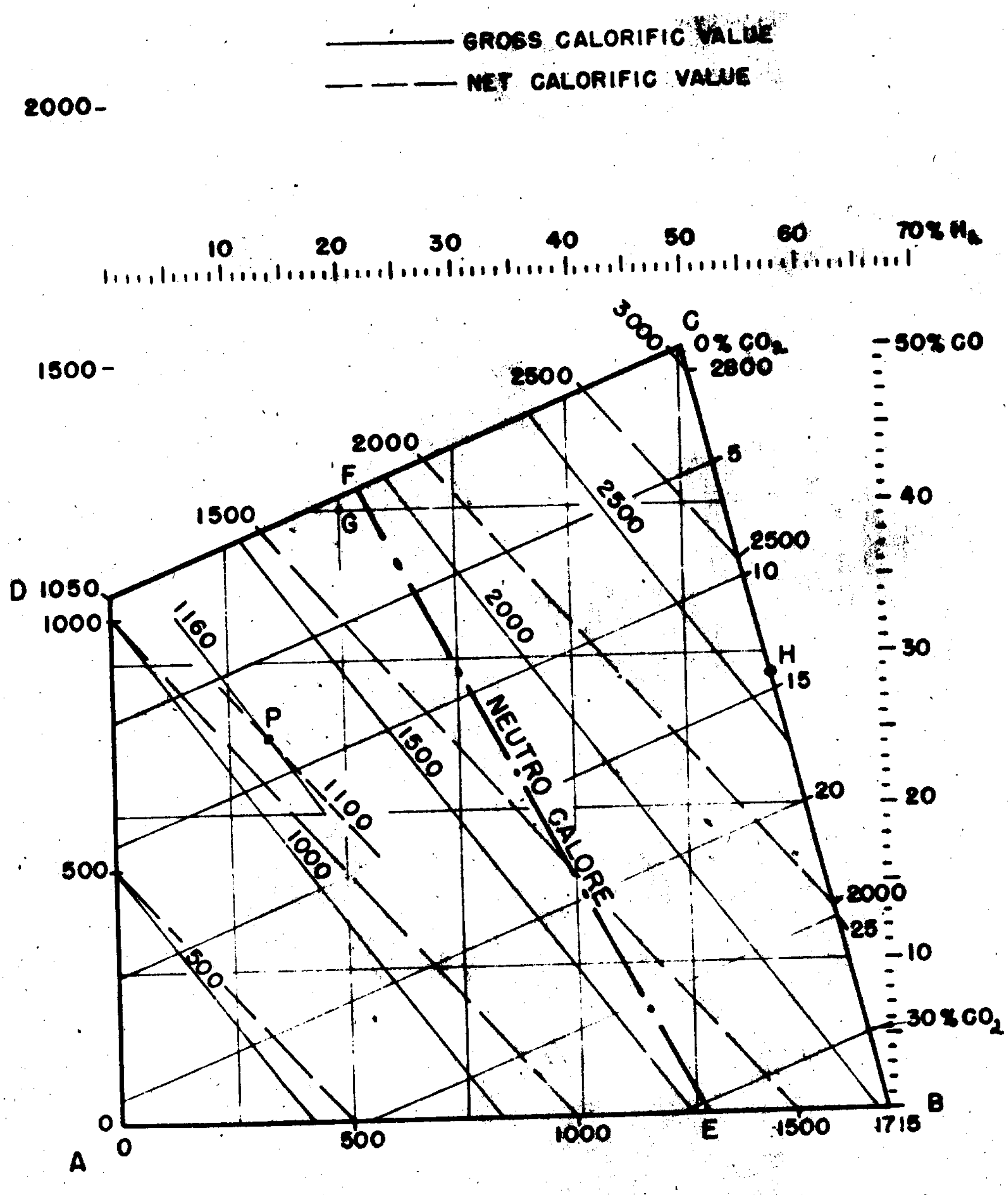

FIG. 8 GROSS AND NET CALORIFIC VALUE OF GASES IN Cal. p. nm.

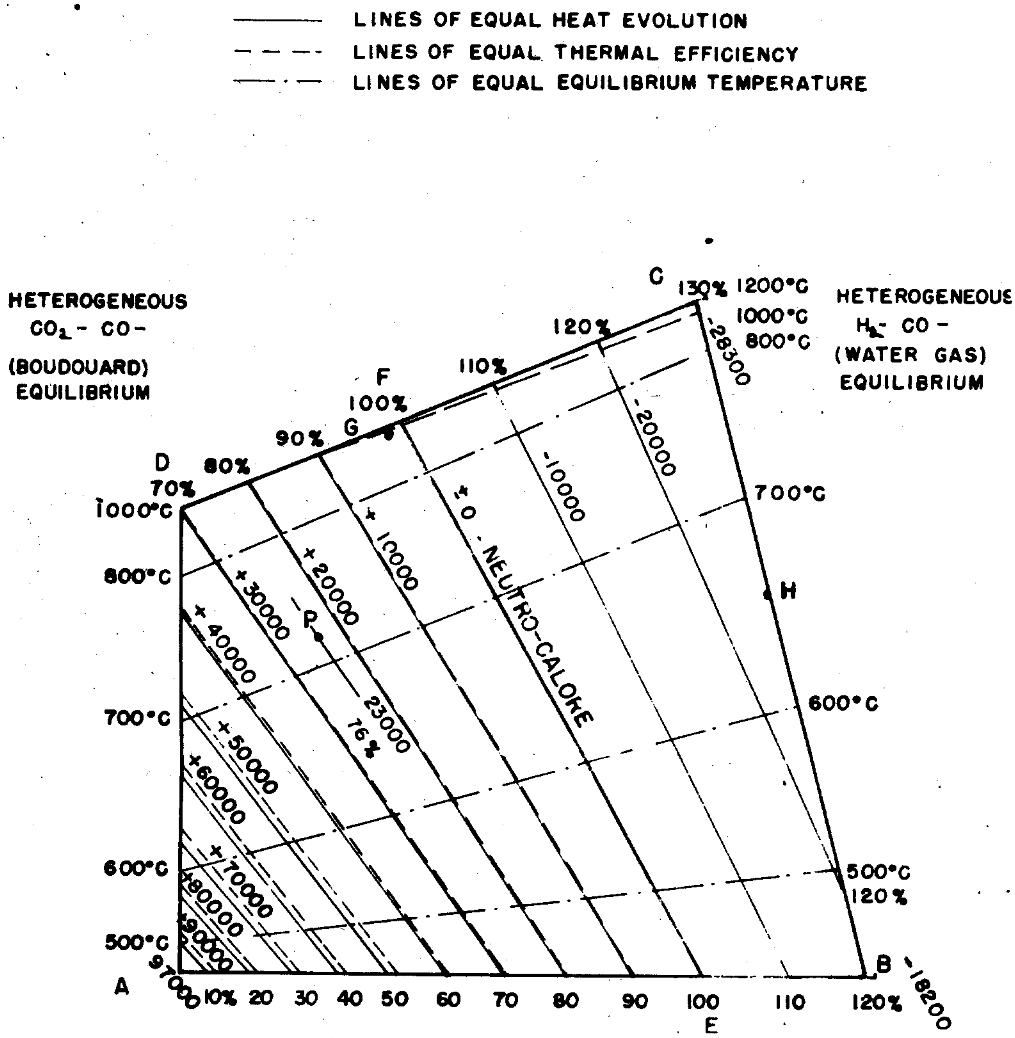

FIG. 9 HEAT EVOLUTION, THERMAL EFFICIENCY, & CHEM. EQUILIBRIUM

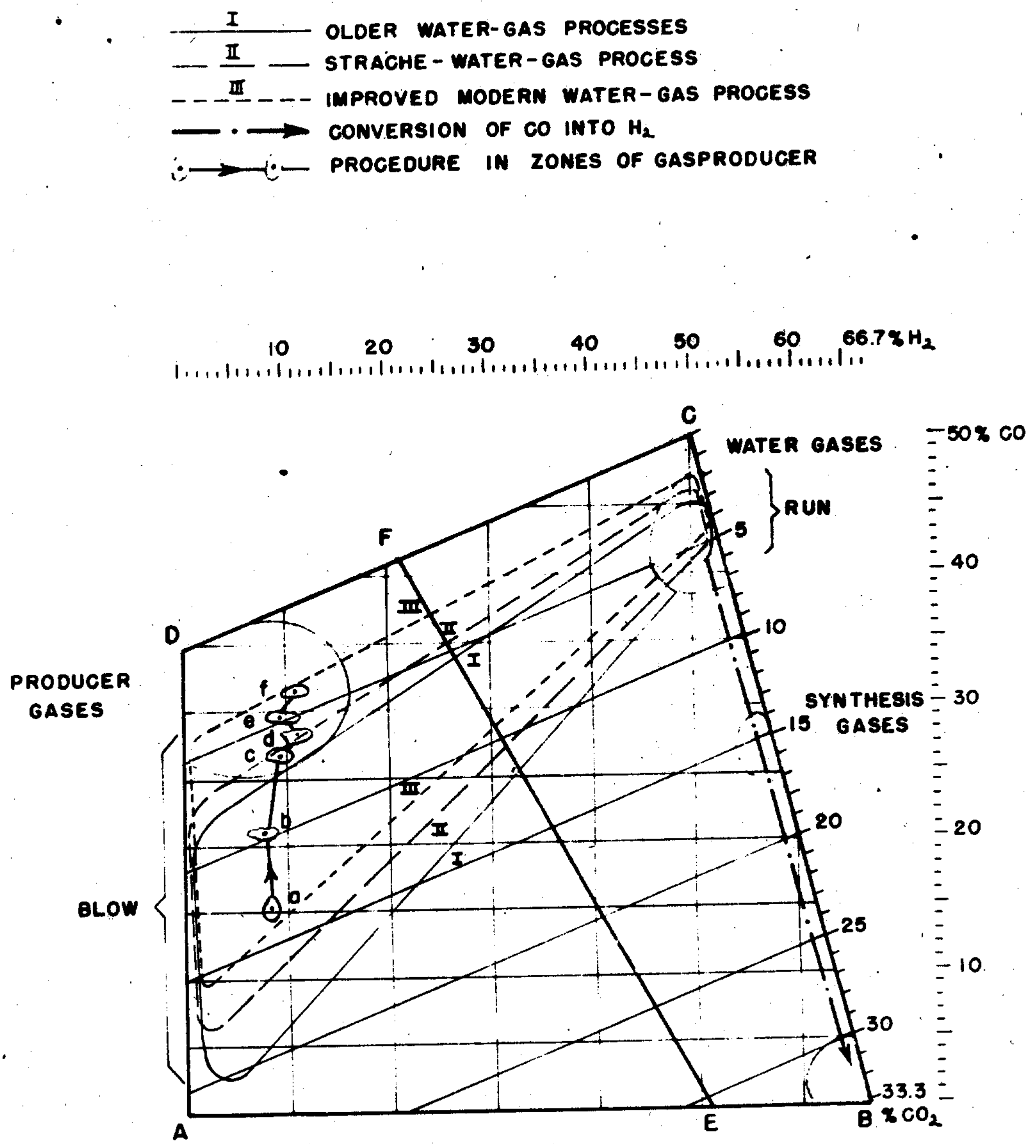

FIG. 10 REPRESENTATIONS OF GASES, PROCEDURES, & PROCESSES