Explanation of Symbols for the Computation of Gas Utilization During the Hydrogenation of Carbon Monoxide.

I. Volumes

CO_2, CO, H_2, CH_4, N_2, - percent of the corresponding gas in the synthesis gas intake.

CO_2', CO', H_2', CH_4', N_2' - percent of these gases in outlet gas.

J, J', - percent of ($CO + H_2$) in the intake or outlet gases.

J_X - proportion of ($CO + H_2$) in synthesis gas which would be completely consumed with a given X, in percent of synthesis gas.

$$p - (CO_2 + CO + CH_4)$$

$$p' - (CO_2' + CO' + CH_4')$$

$$q - 2/(2CO_2 + CO) - (H_2 + 2CH_4)/$$

$$q' - 2/(2CO_2' + CO') - (H_2' + 2CH_4')/$$

R - residual volumes of the outlet reaction outlet gases from one volume of synthesis gas

R_1 - measured residual volume

R_2 - measured residual volume recalculated to normal conditions

R_3 - residual volume calculated from N_2 and N_2'

R_4 - residual volume calculated from precision determinations of N_2'

R_5 - residual volume calculated from gas analyses for $n = 2.0$

R_6 - residual volume calculated from gas analyses with the value for n found from the analyses of the products.

R_7 - residual volume calculated from gas analysis and an assumed value for n.

a - carbon monoxide consumed

b - hydrogen consumed

c - methane formed

c^* - higher hydrocarbons formed, without methane

c_m - total hydrocarbons formed, including methane

d - carbon dioxide formed

e - water formed

d_1, e_1 - volumes of carbon dioxide or water found as such

d_2, e_2 - volumes of carbon dioxide or steam calculated for the formation of pure hydrocarbons

^{x} symbol for proportion of substances chemically or physically bound, or set free.

d^x carbon dioxide liberated or combined.

a, b, c, d and e: volumes of the corresponding gases used up or formed per unit volume of the intake synthesis gas, or in computations with the numerical results of gas analysis per hundred volumes of the intake synthesis gas.

E^x_o cubic meters of synthesis gas intake during the time interval measured, calculated to normal state.

II Characteristic Numbers

U: $(CO + H_2)$ Conversion, in percent of J.

Uco: CO conversion in percent of CO.

Mv: $(CO + H_2)$ consumption for the formation of CH_4, intotal percent of $(CO + H_2)$.

Mco: CO as CH_4, in percent of the CO consumed.

X: Ratio of hydrogen consumed: carbon monoxide consumed.

A: Yields, in g/cbm of synthesis gas.

A_1 - A_9 yields of hydrocarbons CH_n, without methane and without oxygen containing products.

A_{10} yield including oxygen-containing products, but without methane, calculated from experimental data.

A_{11} yield including oxygenated products, calculated from A_1 to A_9 with respect to oxygen containing groups.

A_{max} 90 maximum theoretically possible yield of higher hydrocarbons without methane with given X and Mv and with 90 percent ($CO + H_2$) conversion.

A_m as before but including methane.

III Dimensionless Factors

n: average value for the atomic proportion hydrogen: carbon.

n: for the total higher hydrocarbons formed without methane for C^+.

n_m: for the total hydrocarbons formed including methane, for C_m.

n_p: for the saturated paraffin hydrocarbons.

n_e: for the CH part, from (ester - 2 mol water).

n_{ald}: for the CH part, from (aldehyde - 1 mol water).

n_s: for the CH part, from (acid - 2 mols water).

C-number: Average C values of the fraction of hydrocarbons passing over in the boiling range of the hydrocarbon fraction.

Z: the average C-number found in the gas analysis for CH_4'.

z: average C number of the hydrocarbons in CH_4' exclusive of pure methane.

β : factor for pure methane in CH_4'.

h: factor for recalculating yield from volumes, CH_n into grams.

k: factors for the calculation of n from the products, indexes the same as for n.

IV. Abbreviations for the Evaluation of Analyses of Liquid Products.

G: total weight of the products formed, without methane.

g: the weight of a fraction distilling in the distillation range of 1 C-number.

(olef) - the amount of olefines in grams, in one fraction.

(par) - grams of paraffin hydrocarbons, in one fraction.

(CH) - grams of CH portion of the oxygen containing compounds of a fraction; indexes and computations as with n.

CH . Z, EZ, NZ, CO . Z - data from the determination of chemical groups for alcohols, esters, acids, and aldehydes.

W": grams of chemically bound water in a fraction, indexes as in n.

Y: amount of chemically combined water in the oxygen containing compounds/cbm of synthesis gas.

Collection of Formulas for the Computation of Gas Utilization in the Hydrogenation of Carbon Monoxide.

I. Generally Applicable Equations

(for any Values of n)

A. Basic Stoichiometric relationships:

1. The first basic stoichiometric relationships:

$$a\,CO + b\,H_2 = c_m\,CH_{n_m} + d\,CO_2 + e\,H_2O$$

Solutions for the first basic equation:

$$c_m = \frac{2(a+b)}{n_m+4} \qquad d = \frac{(n_m+2)\,a - 2b}{n_m+4} \qquad e = \frac{4b - n_m a}{n_m+4}$$

2. The second basic stoichiometric equation:

$$aCO + bH_2 = c^{+}CH_n + cCH_4 + dCO_2 + eH_2O$$

Solutions for the second basic equation:

$c^{+}_{1} = \frac{2}{n + 4} (a + b - 4c)$ $c^{+}_{2} = a - c - d$ $c^{+}_{3} = \frac{2}{4 - n} \cdot (3a - b - 4d)$

$c^{+}_{4} = \frac{2}{n + 3} \cdot (b + d - 3c)$ $d_{2} = \frac{n(a - c) + 2(a - b) + 4c}{n + 4}$

$$e = \frac{n(2c - a) + 4b - 8c}{n + 4}$$

B. Intermediate values:

$a = CO - R \cdot CO'$ $b = H_2 - R \cdot H_2'$ $c = R \cdot CH_4' - CH_4$

$d_1 = R \cdot CO_2' - CO_2$ $a + b = J - R \cdot J' = J \cdot U \cdot 10^{-2}$

C. Calculation of n and R:

1. $R_2 = \frac{N_2}{N_2'}$

2. The n - R equations for the first basic stoichiometric equation.

   1. $p_m = CO_2 + CO$ $q_m = 2(2CO_2 + CO - H_2)$

      $p'_m = CO_2' + CO'$ $q'_m = 2(2CO_2' + CO' - H_2')$

      $n_m = \frac{q'_m \cdot R - q_m}{p_m - p'_m \cdot R}$ $R = \frac{q_m + p_m \cdot n_m}{q'_m + p'_m \cdot n_m}$

3. The n - R equation from the second basic stoichiometric equation:

   $p = (CO_2 + CH_4 + CO)$ $q = 2/(2CO_2 + CO) - (H_2 + 2CH_4)/$

   $p' = CO_2' + CH_4' + CO'$ $q' = 2/(2CO_2' + CO') - (H_2' + 2CH_4')/$

   $n = \frac{q' R - q}{p - p' R}$ R_6 or $R_7 = \frac{p \cdot n + q}{p' \cdot n + q'}$

4. n from the intermediate values

$$n = 2 \frac{(b + 2d) - (a + 2c)}{a - (c + d)}$$

5. Recalculating n into n_m:

$$n_m = \frac{c^{+} \cdot n + 4c}{c^{+} + c} = n + c \frac{4 - n}{a - d} = 2 \cdot \frac{(b + 2d - a)}{a - d}$$

D. Calculation of the Characteristic Numbers:

1. Conversion and ratio of consumption

$$U = \frac{a - b}{a} \cdot 10^2$$

$$X = \frac{b}{a}$$

2. Methane formation

$$Mv = \frac{4c}{a + b} \cdot 10^2 \qquad Mco = \frac{c}{a} \cdot 10^2 \qquad Mv = Mco \frac{4}{1 + X}$$

$$= \frac{z - Z}{z - 1} \qquad \text{for} \quad z = Z + 1, \qquad \beta = \frac{1}{Z}$$

E. Calculations of Yields:

1. Higher hydrocarbon yields without methane:

$$A_1 = \frac{12 + n}{22.4} \cdot \frac{2}{n + 4} \; (a + b - 4c) \cdot 10 = h_1 \; (a + b - 4c)$$

$$A_2 = \frac{12 + n}{22.4} \cdot (a - c - d) \cdot 10 \qquad = h_2 \cdot (a - c - d)$$

$$A_3 = \frac{12 + n}{22.4} \cdot \frac{2}{4 - n} \; (3a - b - 4d) \cdot 10 = h_3 \; (3a - b - 4d)$$

$$A_4 = \frac{12 + n}{22.4} \cdot \frac{2}{n + 2} \; (b - 3c + d) \cdot 10 \; = h_4 \; (b - 3c + d)$$

$$A_1 = h_1 \cdot (a + b) \; (100 - Mv) \cdot 10^{-2}$$

$$A_3 = h_3 \; (a + b) \; (1 \; \frac{Mco}{25(1 + X)}) \cdot 10^{-2}$$

$$A_4 = 0.393 \; / 5a + b - 4(2c + d) /$$

2. Maximum theoretical yield:

$J_X = CO \; (1 + X)$, when H_2 in entering gas in excess over H_2 in J_X

$J_X = H_2 \; (\frac{1 + X}{X})$, when CO in entering gas in excess over CO in J_X

$A_{max}\ 90 = h_1 \cdot \bar{J}_X \cdot 90\ (100 - Mv) \cdot 10^{-4}$

3. Hydrocarbon yield including methane:

$$A_{1m} = \frac{20\ (12 + n_m)}{22.4\ (4 + n_m)}\ (a + b) \qquad = h_1\ (a + b)$$

$$A_{2m} = \frac{10\ (12 + n_m)}{22.4}\ (a - d) \qquad = h_2\ (a - d)$$

$$A_{6m} = \frac{20\ (12 + n_m)}{22.4\ (2 + n_m)}\ (b + d) \qquad = h_6\ (b + d)$$

$$A^{1}_{7m} = \frac{20}{22.4}\ (5a + b - 4d) \qquad 0.893\ (5a + b - 4d)$$

4. Numerical values for the factor h:

n or n_m	h_1	h_2	h_5	h_6
2.0	2.083	6.250	6.250	3.125
2.05	2.074	6.272	6.433	3.097
2.10	2.064	6.295	6.649	3.071
2.15	2.054	6.316	6.829	3.044
2.20	2.045	6.339	7.044	3.019
2.25	2.036	6.361	7.270	2.994
2.30	2.027	6.383	7.511	2.969
2.35	2.018	6.406	7.765	2.946
2.40	2.009	6.422	8.036	2.922

5. Yield of total products (higher hydrocarbons and oxygen-containing products, without methane).

$$A_{10} = \frac{G}{E} \qquad A_{11} = A_1\ (\text{or } A_2 \text{ to } A_7) + Y$$

F. Testing the Formation of Carbon Dioxide:

$d'' = d_1 - d''$, calculated with R_1, R_2, R_5 or R_4, and with $n = 2.15$ ($\pm$ 0.15).

II Approximation Equations for n = 2.0

1. Solutions for the first basic stoichiometric equation.

$$c_m = \frac{1}{3}(a + b) \qquad d = \frac{1}{3}(2a - b) \qquad e = \frac{1}{3}(2b - a)$$

2. Solutions for the second basic stoichiometric equation.

$$c^{+} = \frac{1}{3}(a + b - 4c) \qquad d = \frac{1}{3}(2a - b + c) \qquad e = \frac{1}{3}(2b - a - 2c)$$

3. Residual volumes.

$$R = \frac{2CO + 3CO_2 - (H_2 + CH_4)}{2CO' + 3CO_2' - (H_2' + CH_4')}$$

$$R = \frac{100 - (4CO_2 + 3CO)}{100 - (4CO_2' + 3CO')}$$

$$R = \frac{300 - (CO + 4H_2 + 4CH_4)}{300 - (CO' + 4H_2' + 4CH_4')}$$

4. Composition of end gas.

$$CO_2' = \frac{1}{R}\left(CO_2 + \frac{/4(2 - X) + \frac{Mv}{100}(1 + X)/ \cdot (100 - 100R)}{36 - 4\,/4(2 - X) + \frac{Mv}{100}(1 + X)/}\right)$$

$$CO' = \frac{1}{R}\left(CO - \frac{3(100 - 100R)}{(1 + 4X) - \frac{Mv}{100}(1 + X)}\right)$$

$$H_2' = \frac{1}{R}\left(H_2 - \frac{3X(100 - 100R)}{(1 + 4X) - \frac{Mv}{100}(1 + X)}\right)$$

$$CH_4' = \frac{1}{R}\left(CH_4 - \frac{3 \cdot \frac{Mv}{100}(1 + X)(100 - 100R)}{4(1 + 4X) - \frac{Mv}{100}(1 + X)}\right)$$