DATA ANALYSIS PROCEDURES IN FISCHER-TROPSCH SYNTHESIS

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Keywords: Fischer-Tropsch, Schultz-Flory, Synthesis

In performing tests on Fischer-Tropsch (F-T) catalysts, it is useful to be able to assess immediately the approximate activity and selectivity of the catalyst with a minimum of information. The procedure described in this paper requires only gas chromatographic data on the gases to and from the reactor. Further, the only gases which need be analyzed are hydrogen, carbon monoxide, methane and carbon dioxide. No flowrate data is needed.
Consider the following reactions:

F-T Reaction (Alkanes) $(2n+1)H_2 + nCO \rightarrow C_nH_{2n+2} + nH_2O$

Water Gas Shift Reaction $H_2O + CO \rightarrow H_2 + CO_2$

Assume the following:

1) The F-T product carbon number distribution can be characterized using a single chain-growth parameter; and
2) The feed gas is comprised of only hydrogen, carbon monoxide and inert gases; and
3) The hydrogen to carbon monoxide ratio in the feed gas, M_f, is known.
4) The relative amounts of hydrogen, carbon monoxide, methane, and carbon dioxide in the tail gas are known.

From assumption 1, the number of moles of hydrocarbon having n carbon atoms can be expressed in the usual manner as:

$$N_n = \alpha^{n-1} N_{CH4}$$

Where N_n and N_{CH4} denote the number of moles of hydrocarbons produced having n and 1 carbon atoms respectively.

Let superscripts f and t denote feed and tail gases. Therefore, from the stoichiometry of the above reactions, the following relationships are apparent:

$$N_{H2}^t = N_{H2}^f - \sum_{n=1}^{\infty} (2n+1)\, N_n + N_{CO2}^t$$

$$= N_{H2}^f - \frac{(3-\alpha)}{(1-\alpha)^2} N_{CH4} + N_{CO2}^t \qquad (1)$$

$$N_{CO}^t = N_{CO}^f - \sum_{n=1}^{\infty} nN_n - N_{CO2}^t$$

$$= N_{CO}^f - \frac{1}{(1-\alpha)^2} N_{CH4} - N_{CO2}^t \qquad (2)$$

Let ϵ represent the overall carbon monoxide conversion:

$$N_{CO}^t = (1-\epsilon)N_{CO}^f \qquad (3)$$

The subscript i represents any component. By dividing equations (1) and (2) by N_{CO}^t, invoking equation (3), and letting the normalized composition be denoted by R's, ($R_i = N_i^t \div N_{CO}^t$) the following equations are obtained:

$$R_{H2} = \frac{M_f}{(1-\epsilon)} - \frac{(3-\alpha)}{(1-\alpha)^2} R_{CH4} + R_{CO2} \qquad (4)$$

$$1 = \frac{1}{(1-\epsilon)} - \frac{1}{(1-\alpha)^2} R_{CH4} - R_{CO2} \qquad (5)$$

Let $Z = 1/(1-\alpha)$. Then equations (4) and (5) can be written as:

$$R_{H2} = \frac{M_f}{(1-\epsilon)} - (2Z^2 + Z)R_{CH4} + R_{CO2} \quad (6)$$

$$\frac{\epsilon}{(1-\epsilon)} = Z^2 R_{CH4} + R_{CO2} \quad (7)$$

Equations (6) and (7) can be solved simultaneously for ϵ and Z:

For $M_f = 2$, $Z = \dfrac{3R_{CO2} + 2 - R_{H2}}{R_{CH4}}$

For $M_f = 2$, $Z = \dfrac{1 + \sqrt{1 - \dfrac{4(M_f-2)}{R_{CH4}}[(M_f - 2)(1+R_{CO2}) + 3R_{CO2} + 2 - R_{H2}]}}{2(M_f - 2)}$

and $\epsilon = \dfrac{Z^2R_{CH4} + R_{CO2}}{(Z^2R_{CH4} + R_{CO2} + 1)}$