

1. Theoretical framework on mathematical expressions

2. Mathematical model for the 1940 pollution

3. Results and discussion

4. Conclusions

J. Oppenheimer

United States
Department of the Interior

Bureau of Mines
Office of Synthetic Liquid Fuels
Research and Development Division
Pittsburgh 13, Pennsylvania

Translations of German Documents on Mathematical Expressions for
Thermodynamic Relationships and the Calculation of Yields
in the Fischer-Tropsch Synthesis

by

R. Brinkley

and

W. Oppenheimer

February, 1947

CONTENTS

	<u>Page</u>
.....	iv
Reel 134, Navy 5811, Item Ib-1, Thermodynamic Expressions	
Formation and Stability of Hydrocarbons	1
.....	1
General considerations	1
Definitions	3
Expressions for cracking and condensation	6
Reel 134, Navy 5811, Item Ib-2, On the Thermodynamics of	
Fischer-Tropsch synthesis	9
Summary	9
Introduction	9
Equilibrium constants	10
Synthesis of butane by the Fischer-Tropsch reaction	13
Effect of introducing an inert gas	17
Effect of introducing water vapor	18
Effect of excess of hydrogen	20
Synthesis of octane by the Fischer-Tropsch reaction	21
Effect of introducing inert gas	23
Effect of introducing water vapor	24
Effect of excess hydrogen	25
Effect of excess CO in the synthesis gas	26
Yield based on hydrogen	27
Discussion of results	28
Conclusion	30
TOM Reel 134, Navy 5811, Item Ib-3, Calculation of Gas Consumption and Synthesis Course in the Hydrogenation of Carbon Monoxide	32
Summary	32
Introduction	32
Introduction to the mathematical procedure	32
Discussion of the notation	33
The residual volume, R	33
Description of characteristic variables	33
Characteristic variables for CO+H ₂ conversion	34
Explanation of selection of symbols	35
Calculations for the hydrocarbon synthesis from gas analysis data	35
Three fundamental rules for all gas analysis calculations	36
Algebraic interpretation of the three rules	37
The two fundamental stoichiometric equations	37
Calculation of the intermediate variables	38
Calculation of the residual volume from the nitrogen content	39
The n-R equation	40

	Page
Application and validity of the correlation between characteristic and intermediate variables	41
Calculation of characteristic variables	45
Conversion and usage ratio	45
Formation of methane	45
Yield of higher hydrocarbons	50
Correlation of hydrogen-carbon ratio and of oxygenated compounds in the products	53
Reasons for extending the evaluations	53
Calculation of Oxygenated groups from gas analysis data	54
Chemical investigation of the products formed	54
Combustion	54
Precise fractional distillation and chemical analysis	55
Application of the formulas derived	58
Evaluation of gas analysis and synthesis data	58
General course of calculations	58
Checking the results	59
Use of work sheets	64
Calculations for the prediction of the course of a synthesis	65
Uniform use of symbols	65
TOM Reel 134, Navy 5211, Item Ib-4, Calculation of Yield for Higher Hydrocarbons, Based on Recent Methods	70
Summary	70
Introduction and explanation of symbols	70
The CO yield	71
Ideal gas yield	71
Limiting yield and fundamental molar constant	72
The fundamental stoichiometric relations	73
The analysis contraction	74
Separation of oxygenated compounds into the CH-radical and water or oxygen	75
Use of abbreviations in formulas	77
Appendix	77

ILLUSTRATIONS

<u>Figure</u>		<u>Following Page</u>
1	Free energy of formation of several paraffin hydrocarbons at 1 atmosphere	2
2	Free energy of formation of several paraffin hydrocarbons at 100 atmospheres	3
3	Free energy of formation of benzene and cyclohexane at 1 atmosphere	4

Following
Page

Free energy of formation of benzene and cyclohexane at 100 atmospheres	4
Free energy of formation of several olefins at 1 atmosphere	5
Free energy of formation of several olefins at 100 atmospheres	5
Free energy of formation of n-octane and cleavage at 1 atmosphere	6
Graphic representation of characteristic variables	34
The yields as functions of the residual volume	45
The β factor for the calculation of pure methane	47

FORWARD

This report is one of a series in the process of compilation by the Office of Synthetic Liquid Fuels, United States Bureau of Pittsburgh, Pennsylvania. Translations of seized German documents are being prepared and grouped in reports according to subject. Two groups of translations concerning Fischer-Tropsch iron catalysts have been issued. These are: "Translations of German Documents on the Development of Iron Catalysts for the Fischer-Tropsch Synthesis - Part I" which includes the following documents:

TOM Reel 101, Document PG-21559-NID

TOM Reel 101, Document PG-21574-NID

TOM Reel 101, Document PG-21581-NID

TOM Reel 101, Document PG-21577-NID

and "Translations of German Documents on the Development of Iron Catalysts for the Fischer-Tropsch Synthesis - Part II", which includes the following documents:

TOM Reel 101, Document PG-21576-NID

TOM Reel 101, Document PG-21578-NID

TOM Reel 101, Document PG-21579-NID

TOM Reel 134, Navy 5811, Item 1b-23 (First Half)

TOM Reel 86, Bag 3979, Item 76.

The present report includes information on thermodynamic relationships and the calculation of yields from gas consumption

Fischer-Sachs Synthesis, described in the following

TOM Reel 134, Navy 5811, Item Ib-1

TOM Reel 134, Navy 5811, Item Ib-2

TOM Reel 134, Navy 5811, Item Ib-3

TOM Reel 134, Navy 5811, Item Ib-4.