

TABLE 4.3-1
FISCHER TROPSCH
MAGNITUDE OF VARIABLE DEPENDENCE

DEPENDENT INDEPENDENT	CO CONVERSION	DEGREE OF POLYMERIZATION	OLEFIN TO PARAFFIN RATIO
K_p ↑↑	↑↑	↑	—
K_H ↑↑	—	↓↓	↓↓
K_o ↑↑	—	↓↓	↑↑

UOP 573-46

TABLE 4.3-2

EFFECT OF TEMPERATURE,
P = 650 psig, H₂/CO = 2.11

PETC Tube-Wall Data

T, °C (°F)	275 (526)	310 (589)	335 (634)
% CO Conversion	30.7	54.8	77.2
Product Distribution, Wt-%:			
C ₁ + C ₂	60.0	67.0	69.7
C ₃	9.9	10.3	10.5
Gasoline (C ₃ = - 204°C)	24.1	20.6	14.2
Diesel (204 - 316°C)	4.3	1.1	3.4
Fuel Oil (316 - 450°C)	1.7	1.0	2.2
Wax (> 450°C)	0	0	0
Gross Molar Flow Rate, (moles/hr x 10 ⁴)	1.51	3.53	6.62

Values Used for Data Fitting

Degree of Polymerization	2.7	2.2	2.1
Olefin-to-Paraffin Ratio	1.0	1.0	1.0

TABLE 4.3-3
TUBE-WALL REACTOR FITTING

Fresh Feed Rate, moles/hr	0.009608
Composition, mol-%	
H ₂ O	0.5
H ₂	66.2
CO	31.0
CO ₂	0.5
CH ₄	1.9
J Factor (SCFH FF/ft ² Cat Surface Area)	23.87
Reactor Dimensions	
Inside Diameter of Tube, ft	0.0402
Outside Diameter of Tube, ft	0.0875
Shell Diameter, ft	0.175
Length, ft	0.5
Catalyst Thickness, ft	0.00208

TABLE 4.3-4

TUBE-WALL FREQUENCY FACTORS

Temp, °C (°F)	275 (526)	310 (589)	335 (634)	Derived Activation Energies (Btu/lb mole)
Frequency Factors				
$k_p^0 [(ft^3_{RX})^2/lb \text{ Cat-hr-mole}]$	73.3	71.5	73.0	26,400
$k_H^0 (ft^3_{RX}/lb \text{ Cat-hr})$	0.436	0.494	0.465	28,800
$k_O^0 (ft^3_{RX}/lb \text{ Cat-hr})$	0.0180	0.0203	0.0193	27,000
$k_{WG}^0 [(ft^3_{RX})^2/lb \text{ Cat-hr-mole}]$	169.58	144.38	170.5	33,000

I = Input

C = Calculated

	I	C	I	C	I	C
% CO Conversion	30.7	30.7	54.8	54.9	77.2	77.2
Degree of Poly.	2.70	2.71	2.20	2.19	2.10	2.10
Olefin/Paraffin	1.00	1.00	1.00	0.988	1.00	0.981
CO + H ₂ Conversion	28.4	27.3	51.1	46.0	66.1	59.2
CO ₂ Molar Flow	1.51 x 10 ⁻⁴	1.50 x 10 ⁻⁴	3.53 x 10 ⁻⁴	3.53 x 10 ⁻⁴	6.62 x 10 ⁻⁴	6.61 x 10 ⁻⁴

Note: All frequency factors are based on a reference temperature of 1100°R.

TABLE 4.3-5

EXAMPLE EXPERIMENTAL RESULTS
STEEL LATHE TURNINGS CATALYST (SLTC) FISCHER-TROPSCH RUNS

Item	Experiment 26 Period C
Catalyst Type	SLTC
Synthesis, hours	416 - 488
Reactor Conditions	
Fresh Feed Rate, scfh	1,214
Space Velocity, vol/vol/hr	607
Reactor Pressure, psig	405
Recycle to Fresh Feed:	
Total	27
Hot	25.5
Cold	1.5
CO ₂ scrubbed	1.5
Reactor Temperature, °F	
In Gas	552
Out Gas	610
Increment	58
Average Catalyst Temperature, °F	586
Maximum Catalyst Temperature, °F	622
H ₂ :CO Ratio, Fresh Gas	1.45
Results	
CO ₂ Free Contraction, %	74.6
H ₂ Conversion, %	73.7
CO Conversion, %	88.7
H ₂ + CO Conversion, %	79.8
H ₂ :CO Ratio:	
Recycle Gas	3.35
Usage	1.21
Water Vapor in Recycle Gas, vol-%	7.0
Tail Gas Composition, vol-%(a)	
H ₂	55.2
CO	16.5
N ₂	1.2
CO ₂	9.6

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TABLE 4.3-5 (Continued)

Item	Experiment 26 Period C
Tail Gas Composition, vol-%(a)	
C ₁	9.8
C ₂ ⁼	0.7
C ₂	2.3
C ₃ ⁼	0.3
C ₃	1.0
C ₄ ⁼	0.6
C ₄	1.8
C ₅ ⁼	0.2
C ₅	0.8
C ₆ ⁼	0
C ₆	0
Yield, g/m ³ (H ₂ + CO) Converted	
C ₁	24
C ₂ ⁼	3
C ₂	12
C ₃ ⁼	2
C ₃	7
C ₄ ⁼	6
C ₄	18
C ₅ ⁼	2
C ₅	9
C ₆ ⁼	0
C ₆	0
Oil	0.97
Aqueous	130
C ₁ - C ₃ OH(b)	8
Other Oxygenates(b)	3
Water	119
CO ₂ 307	
Hydrocarbon Recovery, g/m ³	191
Theoretical Recovery, g/m ³	201
Hydrocarbon Recovery, wt-%	
C ₁ + C ₂	19.4
C ₃	3.5
Gasoline (C ₃ = < 400°F)	59.0
Diesel Oil (400 to 600°F)	9.1
Fuel Oil (600 to 842°F)	6.2
Wax (< 842°F)	2.8

(a) Dry basis.

(b) Calculated as hydrocarbons.

TABLE 4.3-6
TUBE-WALL vs. LATHE TURNINGS
FREQUENCY FACTORS

	<u>Tube-Wall</u>	<u>Lathe Turning</u>	<u>Adjusted Lathe Turning</u>
k_p^0 [(ft ³ _{Rx}) ² /lb Cat-hr-mole]	73.0	113.0	73.0
k_H^0 (ft ³ _{Rx} /lb Cat-hr)	0.465	0.108	0.070
k_O^0 (ft ³ _{Rx} /lb Cat-hr)	0.0193	0.002	0.0013
k_{WG}^0 [(ft ³ _{Rx}) ² /lb Cat-hr-mole]	170.0	318.0	205.0

Note: All frequency factors are based on a reference temperature of 1100°R.

TABLE 4.3-7

OPERATING DATA AND RESULTS OF LIQUID-PHASE SYNTHESIS FOR ONE-STEP OPERATION
WITH A SINGLE PASSAGE OF THE GAS OVER IRON CATALYSTS

Effective Reaction Space, volume suspension including dispersed gas, (λ)	10,000
Catalyst, kg Fe	800
Synthesis Gas Pressure, bar	12
Synthesis Gas, (volume ratio, CO:H ₂)	1.5
Quantity of Synthesis Gas, Nm ³ /h	2700
Linear Velocity of the Compressed Gases at Operating Temperature Referred to the Free Reactor Cross Section, cm/s	9.5
Total CO + H ₂ used, Nm ³ /h	2300
per m ³ of Reaction Chamber	230
per kg of Fe	2.6
Average Synthesis Temperature, °C	268
CO Conversion, %	91
CO + H ₂ Conversion, %	89
Synthesis Products Referred to CO + H ₂ used, g/Nm ³	
Hydrocarbons	
C ₁ +	178
C ₁ + C ₃	12
C ₃ +	166
O-containing Products in the Synthesis Water, g/Nm ³	3
Space-time Yield of C ₃ + Products incl. O-products in 24 hours (kg/m ³ of reaction chamber)	930

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TABLE 4.3-7 (Continued)

Composition of a Product from the Demonstration Plant
(Mode of Operation Adjusted for Gasoline Production)

	<u>CO + H₂, g/Nm³</u>	<u>Wt-% of Total Product C₁+</u>	<u>Olefin, %</u>
Methane + Ethane	5.7	3.2	0
Ethylene	613	3.6	100
C ₃	40.3	22.6	75-85
C ₄	9.1	5.1	70-80
40-180°C Fraction	95.5	53.6	70
180-220°C	7.1	4.0	48
220-320°C	10.7	6.0	37
> 320°C	3.3	1.9	7
Total	178.0	100.0	

TABLE 4.3-8

SLURRY AND ENTRAINED BED INPUT
FOR FITTING PURPOSES

Fresh Feed Rate, moles/hr Composition, %	Slurry 251.6	Entrained Bed 86,585.9
H ₂ O	3.0	0.01
H ₂	38.0	66.51
CO	54.0	27.71
CO ₂	5.0	5.77
Recycle Rate, moles/hr Composition	-	192,500.00
H ₂ O		0.37
H ₂		4.78
CO		2.83
CO ₂		26.82
Cl		16.92
n-C ₂		3.90
n-C ₃		1.19
n-C ₄		0.52
n-C ₅		0.15
n-C ₆		0.03
n-C ₇		0.0081
n-C ₈		0.0017
n-C ₉		0.0005
n-C ₁₀		0.0002
=C ₂		3.72
=C ₃		4.50
=C ₄		2.72
=C ₅		1.05
=C ₆		0.33
=C ₇		0.115
=C ₈		0.034
=C ₉		0.0115
=C ₁₀		0.0038
Pressure, psia	174	380 (inlet)
Temperature, °F	514	599 (inlet)
Space Velocity, $\frac{\text{SCFEE}}{\text{hr-ft}^3 \text{ reactor}}$	280	959
Catalyst Concentration (lbs cat/ft ³ slurry)	4.44	-
$\frac{\text{lbs cat circulated}}{\text{sec.}}$	-	26,057

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TABLE 4.3-8 (Continued)

Total Reactor ΔT , °F	-	36
% CO Conversion, FF	91	97.8
Degree of Polymerization	4.0	3.3
Olefin-to-Paraffin Ratio	1.0	1.0
Gross CO ₂ Molar Flow, moles/hr	73.4	5,133.6

TABLE 4.3-9

FREQUENCY FACTOR COMPARISON

<u>Frequency Factor</u>	<u>Tube-Wall</u>	<u>Lathe Turning</u>	<u>Slurry</u>	<u>Entrained Bed</u>
$k_p^0 [(ft^3_{RX})^2/1b \text{ Cat-hr-mole}]$	73.0	113.0	2604.0	1821.0
$k_H^0 (ft^3_{RX}/1b \text{ Cat-hr})$	0.465	0.106	3.94	1.11
$k_o^0 (ft^3_{RX}/1b \text{ Cat-hr})$	0.0193	0.002	0.06	0.015
$k_{WG}^0 [(ft^3_{RX})^2/1b \text{ Cat-hr-mole}]$	170.0	318.0	10,699.0	228.8

NORMALIZED FOR SURFACE AREA PER POUND
OF CATALYST DIFFERENCES USING
TUBE-WALL AS BASE

<u>Frequency Factor</u>	<u>Tube-Wall</u>	<u>Lathe Turning</u>	<u>Slurry</u>	<u>Entrained Bed</u>
$k_p^0 [(ft^3_{RX})^2/1b \text{ Cat-hr-mole}]$	73.0	73.0	73.0	73.0
$k_H^0 (ft^3_{RX}/1b \text{ Cat-hr})$	0.465	0.070	0.110	0.045
$k_o^0 (ft^3_{RX}/1b \text{ Cat-hr})$	0.0193	0.00129	0.0016	0.0006
$k_{WG}^0 [(ft^3_{RX})^2/1b \text{ Cat-hr-mole}]$	170.0	205.0	300.0	9.2

Note: All frequency factors are based on a reference temperature of 1100°R.

TABLE 4.3-10

EXAMPLE EXPERIMENTAL RESULTS
FLAME SPRAYED CATALYST (FSC) FISCHER-TROPSCH RUNS

<u>Item</u>	<u>Experiment No. HGR 33</u>		<u>Experiment No. HGR 34</u>	
Catalyst Type	Coated Plates	Coated Plates	Coated Plates	Coated Plates
Fresh Gas Velocity, vol/vol/hr	600	1000	1000	2000
Fresh Feed Rate, scfh	165	275	275	550
Recycle Ratio				
Total Recycle:Fresh Feed, vol/vol	51	15.9	20.4	14.4
Reactor Pressure, psig	400	400	400	400
Catalyst Temperature, °F				
Average	516	617	608	617
Differential	36	90	72	90
H ₂ Conversion, %	73.4	90.9	90.1	83
CO Conversion, %	80.6	98.8	98.2	94.4
H ₂ + CO Conversion, %	76.4	94.4	93.4	87.5
Overall Weight Balance, %	93.6	90.8	87.8	96.6
Hydrocarbons Recovered lb/1,000 scf fresh gas	7.4	9.5	10.3	11.6
Hydrocarbons Recovered, wt-%				
C ₁ + C ₂	59.7	36.5	33.9	29.5
C ₃	6.6	14.1	13.3	12.8
Gasoline (C ₃ = < 400°F)	31.8	43.7	48.5	53.0
Diesel Fuel (400 to 600°F)	1.9	5.0	4.0	3.8
Fuel Oil (600 to 842°F)	0	0.4	0.2	0.5
Wax (> 842°F)	0	0.3	0.1	0.4

TABLE 4.3-11

KEY REACTOR DESIGN BASIS ELEMENTS

Capacity, Btu/day Total Products HHV, billion	500
Pressure, psig	400
Temperature (average), °F	606
Space Velocity Factors	
J, scf/hr/sq ft of catalyst area	10
S _v , scf/hr/cu ft of reaction zone volume	1,330
Catalyst Activity	1.33
Syngas Composition	
Fresh Feed H ₂ :CO Ratio	1.45
CO + H ₂ Conversion, %	80
Reactor Recycle Ratio	
Volume Recycle Gas : Volume (CO + H ₂) in Fresh Syngas Feed	1.5
Heat of Reaction at Reactor Conditions	
Btu/scf of (CO + H ₂) Converted	72.8

REACTOR PRODUCT COMPOSITION

	Weight Percent
C ₁ , C ₂ , C ₂ ⁻	19.3
C ₃ , C ₃ ⁻	4.5
C ₄ , C ₄ ⁻	11.9
C ₅ , C ₅ ⁻ , C ₆	13.6
C ₇ , C ₈ , C ₉	19.2
C ₁₀ , C ₁₁ to 640°F BP	18.8
640 to 940°F BP	7.3
Alcohols and Ketones	4.9
Acids	0.5
Total	<u>100.00</u>

TABLE 4.3-12

CONCEPTUAL FISCHER-TROPSCH REACTOR DESIGN
COMPARED WITH PETC EXPERIMENTAL DATA

<u>Item</u>	<u>Experiment HGR 34</u>		<u>SLTC Experiment 26C</u>	<u>TWR Experiment FT-TW-1</u>	<u>Conceptual Design Basis</u>
"J", scfh/sf Catalyst Surface	8.85	17.7	1.5	30	10.0
H ₂ :CO Ratio in Feed	1.41	1.41	1.45	3	1.45
Recycle Ratio	20.4	14.4	27.0	-	1.5
(CO + H ₂) Conversion, %	93.4	87.5	80.0	52.0	80.0
Total Reaction Heat Calculated, Btu/sf/hr	583.0	1092.0	84.0	1100.0	563.0

TABLE 4.3-13

TUBE-WALL REACTOR DESIGN COMPARISON

<u>OPERATING CONDITIONS</u>	<u>Parsons</u>	<u>UOP Model Prediction</u>	
Case	Study	<u>1</u>	<u>2</u>
Inlet Temperature, °F	571	571	606
Coolant Temperature, °F	606	606	640
Pressure, psia	415	415	415
J Factor (FF), ft ³ /hr-ft ²	10.0	10.0	5.38
GHSV (FF), hr ⁻¹	1330	1331	716.2
Recycle Ratio	1.5	1.5	1.5
H ₂ /CO Ratio			
Fresh Feed	1.45	1.45	1.45
Combined Feed	2.17	2.17	2.03
Catalyst	Flame sprayed magnetite	K promoted, flame sprayed taconite	
<u>YIELD INFORMATION</u>			
CO Conversion, mol-%			
Fresh Feed	88.7	34.9	90.0
Combined Feed	55.6	21.9	54.4
Degree of Polymerization	4.30	5.92	4.30
CO + H ₂ Conversion, mol-%	53.3	18.8	41.1

TABLE 4.3-14
INFLUENCE OF RECYCLE TO FEED RATIO
ON COMPONENT CONCENTRATIONS
IN COMBINED FEED

RUN	1-T	5	32
Recycle/Feed	0	1.0	2.5
Mole Fraction in Combined Feed			
H ₂	0.645	0.69	0.69
CO	0.323	0.23	0.21
Total Olefins	0	0.008	0.016
% CO Conversion (on Fresh Feed)	89.5	86.7	86.2
Degree of Polymerization	4.78	4.23	4.24

TABLE 4.3-15
SLURRY OPERATING CONDITIONS

	<u>Koelbel</u>	<u>Base Case</u>
GHSV (Hr ⁻¹)	262	453
Pressure (psia)	174	300
H ₂ /CO Ratio	0.7	0.7
Temperature (°F)	514	514
CO Conversion (%)	91	91

TABLE 4.3-16
COMPARISON OF SINGLE-STAGE
AND TWO-STAGE SLURRY REACTOR

	<u>Single- Stage</u>	<u>Two-Stage 1st Length</u>	<u>Total</u>
Reactor Length (Ft)	26.0	15.0	26.0
Reactor Diameter (Ft)	4.22	4.22	4.22
GHSV (Hr ⁻¹) (FF)	262.4	453.2	262.4
Temperature (°F)	514	514	514
Pressure (psia)	174	174	174
H ₂ /CO (Product)	1.8	1.20	2.92
CO Conversion (%)	91	78	95
Degree of Polymerization	4.0	5.4	4.7

TABLE 4.3-17

YIELDS VERSUS REACTOR LENGTH

Tube-Wall Reactor

 H_2/CO , FF = 2.0

Once Through

Temperature, °F = 640

CO Conversion = 98.3%

Pressure, psig = 415

Relative Reactor Position	0	0.2	0.8	1.0
Yields				
H_2 (Mole Fraction)	0.645	0.522	0.406	0.374
CO (Mole Fraction)	0.323	0.133	0.012	0.010
Total Olefins	0	0.017	0.029	0.030
Degree of Polymerization	6.01	4.70	4.32	4.32

TABLE 4.3-18
REACTOR BASE COMPARISON

	<u>Tube-Wall</u>		<u>Slurry</u>	<u>Entrained Bed</u>
J Factor	5	10	1.9	1.2
GHSV (hr ⁻¹)	103	241	280	959
B (SCF/lb Cat/Hr)	10	20	90	58
Temp (°F)	590	660	514	616*
Pressure (psig)	400	400	159	365**
H ₂ /CO mol ratio (FF)	2.0	2.0	0.7	2.4
H ₂ /CO mol ratio (CF)	-	-	-	4.23
Recycle Ratio	-	-	-	2.36
% CO Conv (FF)	89.5	89	91	97.8
% CO Conv (CF)	-	-	-	79.7
DP	4.78	4.4	4.0	3.3

* Mean Temperature [(Inlet + Outlet)/2]

** Inlet Pressure

TABLE 4.3-19

REACTOR COMPARISON

	<u>Base</u>		<u>Per Mole CO + H₂ Used</u>			
	<u>Tube- Wall</u>	<u>Entrained Bed</u>	<u>Slurry</u>	<u>Tube- Wall</u>	<u>Entrained Bed</u>	<u>Slurry</u>
<u>Moles H₂ Converted</u> <u>Mole FF</u>	0.35	0.60	0.29	<u>Moles H₂</u> <u>Mole CO + H₂</u> Used	0.55	0.69 / 0.37
<u>Moles CO Converted</u> <u>Moles FF</u>	0.29	0.27	0.49	<u>Moles CO</u> <u>Mole CO + H₂</u> Used	0.45	0.31 0.63
<u>Mole H₂O Produced</u> <u>Mole FF</u>	0.12	0.27	0.0084	<u>Moles H₂O</u> <u>Mole CO + H₂</u> Used	0.19	0.31 0.011
<u>Moles CO₂ Produced</u> <u>Mole FF</u>	0.09	0.0	0.24	<u>Moles CO₂</u> <u>Mole CO + H₂</u> Used	0.14	0.0 0.31
<u>Lbs HC Produced</u> <u>Mole FF</u>	2.90	3.92	3.56	<u>Lbs HC</u> <u>Mole CO + H₂</u> Used	4.53	4.51 4.56