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APPENDIX A

DERIVATION OF REACTION MECHANISM

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APPENDIX A

DERIVATION OF PRODUCT RATE EQUATIONS

The derivation of product rate expressions proceeds as follows. The rate of formation of the active species,  $M(CH_2)H$ , can be described by the following equation:

$$r_{M(CH_2)H} = k_p[MH][CO][H_2] - k_p[M(CH_2)H][CO][H_2] - k_H[M(CH_2)H][H_2] \quad (1)$$

$M(CH_2)H$  can be defined in terms of  $MH$  with the assumption of steady state:

$$[M(CH_2)H] = \frac{k_p[CO][H_2]}{k_p[CO][H_2] + k_H[H_2]} [MH] \quad (2)$$

In order to simplify the equations, let  $D = k_p[CO][H_2]$ ,  $E = k_H[H_2]$  and  $C = D/(D + E)$ . This equation then simplifies to:

$$[M(CH_2)H] = C [MH] \quad (3)$$

In a similar manner, the rate of formation of  $M(CH_2)_nH$  is described as:

$$r_{M(CH_2)_nH} = 0 = D [M(CH_2)_{n-1}H] - D [M(CH_2)_nH] - E [M(CH_2)_nH] - k_o [M(CH_2)_nH] + \frac{k_o}{K_e} [C_nH_{2n}][MH] \quad (4)$$

If one now collects terms and sets  $A = D/(k_o + D + E)$  and  $B = k_o/K_e$  ( $k_o + D + E$ ), and solves for  $[M(CH_2)_nH]$ , the following equation results:

$$[M(CH_2)_nH] = A [M(CH_2)_{n-1}H] + B [C_nH_{2n}][MH] \quad (5)$$

Using the method of successive substitution, Equations 3 and 5 lead to:

$$[M(CH_2)_nH] = A^{n-1} C + B \sum_{i=2}^n A^{n-i} [C_iH_{2i}] [MH] \quad (6)$$

Substituting Equations 6 and 3 into Equation 1 and rearranging gives:

$$[MH] = \frac{[CAT]}{1 + C + \sum_{j=2}^n \left( A^{j-1} C + B \sum_{i=2}^j A^{j-i} [C_iH_{2i}] \right)} \quad (7)$$

Rate expressions for the products can be written as follows:

Methane

$$r_{CH_4} = k_H [M(CH_2)H] [H_2] \quad (8)$$

Paraffins  $n \geq 2$

$$r_{C_nH_{2n+2}} = k_H [M(CH_2)_nH] [H_2] \quad (9)$$

Olefins  $n \geq 2$

$$r_{C_nH_{2n}} = k_o [M(CH_2)_nH] - \frac{k_o}{K_e} [C_nH_{2n}] [MH] \quad (10)$$

Substitution for  $[M(CH_2)_nH]$  in these expressions leads to the final product rate expressions:

Methane

$$r_{CH_4} = C k_H [H_2] [MH] \quad (11)$$

Paraffins  $n \geq 2$

$$r_{C_nH_{2n+2}} = \left( A^{n-1} C + B \sum_{i=2}^n A^{n-i} [C_iH_{2i}] \right) k_H [H_2] [MH] \quad (12)$$

Olefins  $n \geq 2$

$$r_{C_nH_{2n}} = \left[ k_o \left( A^{n-1} C + B \sum_{i=2}^n A^{n-i} [C_iH_{2i}] \right) - \frac{k_o}{K_e} [C_nH_{2n}] \right] [MH] \quad (13)$$

APPENDIX B

REACTOR MODELING INPUT CHECKLIST

APPENDIX B  
INPUT PARAMETERS

<u>Parameter</u>	<u>Tube- Wall</u>	<u>Entrained Bed</u>	<u>Slurry</u>
<b>I. Indicators</b>			
A. Number of Components	X	X	X
B. Number of Stages in Gas Phase	X	X	X
C. Number of Stages in Liquid Phase			X
D. Number of Reactions	X	X	X
E. Number of Olefin Forming Reactions	X	X	X
F. Number of Paraffin Forming Reactions	X	X	X
G. Number of Reactors	X	X	X
H. Temperature Mode Indicator	X	X	
I. Kinetic Mechanism Selector	X	X	
J. Predict or Convergence Indicator	X	X	
K. Type of Tubular Reactor	X		X
L. Carbon Number Indicators for Degree of Polymerization Calculation	X	X	X
M. Carbon Number Indicator for Olefin-to-Paraffin Ratio Calculation	X	X	X
<b>II. Reactor Information</b>			
A. Number of Tubes	X	X	
B. Tube Diameter			
1) Inside	X		
2) Outside	X		
C. Tube Thickness	X		
D. Shell Diameter	X		
E. Reactor Diameter		X	X
F. Reactor Length	X	X	X
<b>III. Operating Parameter</b>			
A. Space Velocity	X		
B. J Factor	X		
C. Inlet Temperature	X	X	X
D. Inlet Pressure	X	X	X
E. Voidage	X		X
F. Mass Transfer Interfacial Area			X
G. Fresh Feed Rate and Composition	X	X	X
H. Recycle Rate and Composition	X	X	X

APPENDIX B (Continued)

INPUT PARAMETERS

<u>Parameter</u>	<u>Tube- Wall</u>	<u>Entrained Bed</u>	<u>Slurry</u>
IV. Catalyst Information			
A. Thickness of Flame-Sprayed Catalyst	X		
B. Catalyst Skeletal Density	X		
C. Catalyst Porosity	X		
D. Ft <sup>2</sup> Catalyst/Ft <sup>3</sup> Reaction Space	X		
E. Slurry Catalyst Loading			X
F. Solids Circulation Rate		X	
V. Fitting Information			
A. CO Conversion	X	X	X
B. Degree of Polymerization	X	X	X
C. Olefin-to-Paraffin Ratio	X	X	X
D. CO <sub>2</sub> Molar Flow Rate	X	X	X
E. Number of Parameters Requiring Fitting			
1) Gas Phase	X	X	X
2) Liquid Phase			X
3) Predict Mode			X
VI. Heat Exchanger Information			
A. Coolant Temperature	X	X	
B. Coolant Designation		X	
C. Coolant Flow Rate		X	
D. Coolant Heat Capacity		X	
E. Exchanger Heights		X	

APPENDIX C

THERMODYNAMIC CONSTANTS

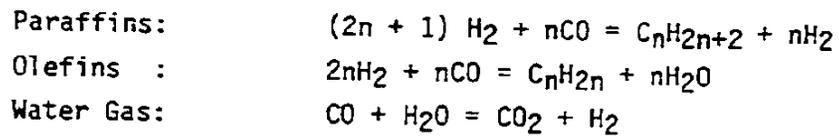
APPENDIX C

I. Heat of Reaction Calculations

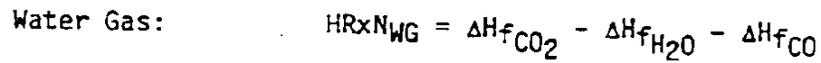
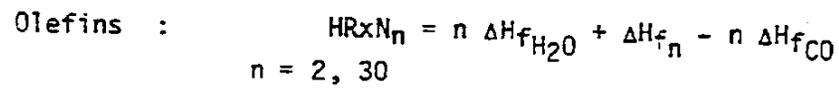
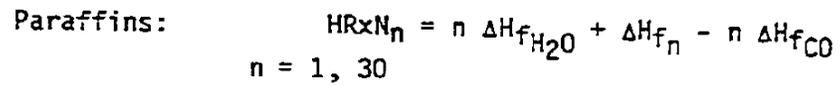
A. Heats of Formation

<u>Component</u>	<u><math>\Delta H_f</math> (Btu/Mole)</u>
H <sub>2</sub> O	-105193.16
H <sub>2</sub>	0.0
CO	-47379.94
CO <sub>2</sub>	-169414.66
C <sub>1</sub> Paraffin	-35542.60
C <sub>2</sub> Paraffin	-41526.08
C <sub>3</sub> Paraffin	-51122.31
C <sub>4</sub> Paraffin	-61967.80
C <sub>5</sub> Paraffin	-72024.86
C <sub>6</sub> Paraffin	-82267.32
C <sub>n</sub> Paraffin n = 7 to 30	$-82267.32 + (n-6)(-5.658)(3.9685)(453.5924)$
C <sub>2</sub> Olefin	+19322.07
C <sub>3</sub> Olefin	+3929.58
C <sub>4</sub> Olefin	-6210.28
C <sub>5</sub> Olefin	-16402.34
C <sub>6</sub> Olefin	-26659.21
C <sub>n</sub> Olefin n = 7 to 30	$-26659.21 + (n-5)(-5.658)(3.9685)(453.5924)$

B. Reactions



C. Heats of Reaction



II. Heat Capacities

A. Equation

$$C_{pI} = A + B \frac{T}{1.8} + C \left( \frac{T}{1.8} \right)^2 \quad (\text{Btu/mole } ^\circ\text{F})$$

where:

$$T = ^\circ\text{R}$$

B. Values for A, B and C

<u>Component</u>	<u>A</u>	<u>B</u>	<u>C</u>
H <sub>2</sub> O	7.256	2.298 x 10 <sup>-3</sup>	-0.283 x 10 <sup>-6</sup>
H <sub>2</sub>	6.947	-0.200 x 10 <sup>-3</sup>	+0.481 x 10 <sup>-6</sup>
C <sub>0</sub>	6.420	1.665 x 10 <sup>-3</sup>	-0.196 x 10 <sup>-6</sup>
C <sub>0</sub> <sub>2</sub>	6.214	10.396 x 10 <sup>-3</sup>	-3.545 x 10 <sup>-6</sup>
C <sub>1</sub> Paraffin	3.381	18.044 x 10 <sup>-3</sup>	-4.300 x 10 <sup>-6</sup>
C <sub>2</sub> Paraffin	2.247	38.201 x 10 <sup>-3</sup>	-11.049 x 10 <sup>-6</sup>
C <sub>3</sub> Paraffin	2.410	57.195 x 10 <sup>-3</sup>	-17.533 x 10 <sup>-6</sup>
C <sub>4</sub> Paraffin	3.844	73.350 x 10 <sup>-3</sup>	-22.655 x 10 <sup>-6</sup>
C <sub>5</sub> Paraffin	4.895	90.113 x 10 <sup>-3</sup>	-28.039 x 10 <sup>-6</sup>
C <sub>6</sub> Paraffin	6.011	106.746 x 10 <sup>-3</sup>	-33.363 x 10 <sup>-6</sup>
C <sub>7</sub> Paraffin	7.094	123.447 x 10 <sup>-3</sup>	-38.719 x 10 <sup>-6</sup>
C <sub>8</sub> Paraffin	8.163	140.217 x 10 <sup>-3</sup>	-44.127 x 10 <sup>-6</sup>
C <sub>n</sub> Paraffin	8.163	140.217 x 10 <sup>-3</sup>	-44.127 x 10 <sup>-6</sup>
	+	+	+
	(n-8)(1.097)	(n-8)(16.667 x 10 <sup>-3</sup> )	(n-8)(-5.338 x 10 <sup>-6</sup> )
C <sub>2</sub> Olefin	2.830	28.601 x 10 <sup>-3</sup>	-8.726 x 10 <sup>-6</sup>
C <sub>3</sub> Olefin	3.253	45.116 x 10 <sup>-3</sup>	-13.740 x 10 <sup>-6</sup>
C <sub>4</sub> Olefin	3.909	62.848 x 10 <sup>-3</sup>	-19.617 x 10 <sup>-6</sup>
C <sub>5</sub> Olefin	5.347	78.990 x 10 <sup>-3</sup>	-24.733 x 10 <sup>-6</sup>
C <sub>6</sub> Olefin	6.399	95.752 x 10 <sup>-3</sup>	-30.116 x 10 <sup>-6</sup>
C <sub>7</sub> Olefin	7.488	112.440 x 10 <sup>-3</sup>	-35.462 x 10 <sup>-6</sup>
C <sub>8</sub> Olefin	8.592	129.076 x 10 <sup>-3</sup>	-40.775 x 10 <sup>-6</sup>
C <sub>n</sub> Olefin	8.592	129.076 x 10 <sup>-3</sup>	-40.775 x 10 <sup>-6</sup>
	+	+	+
	(n-8)(1.097)	(n-8)(16.667 x 10 <sup>-3</sup> )	(n-8)(-53.380 x 10 <sup>-6</sup> )

APPENDIX D

DERIVATION OF SLURRY MASS TRANSFER/MASS BALANCE

APPENDIX D

DERIVATIONS OF SLURRY MASS TRANSFER  
MASS BALANCE EQUATIONS

The basic mass balance equation is:

$$-\frac{1}{A} \frac{d(V_G Y_i)}{dZ} = k_{L_i} a C_L \left( \frac{Y_i}{K_i} - X_{b_i} \right) \quad (1)$$

where:

- A = reactor cross sectional area (ft<sup>2</sup>)
- V<sub>G</sub> = molar flow rate (moles/hr)
- Y<sub>i</sub> = gas mole fraction of component i
- Z = reactor length (ft)
- k<sub>L<sub>i</sub></sub> = mass transfer rate constant for component i (ft<sup>3</sup> liq/ft<sup>2</sup>-hr)
- a = interfacial area (ft<sup>2</sup>/ft<sup>3</sup> reactor)
- C<sub>L</sub> = liquid molar concentration (moles/ft<sup>3</sup> liq)
- K<sub>i</sub> = vapor-liquid equilibrium constant
- X<sub>b<sub>i</sub></sub> = bulk liquid mole fraction of component i

This equation can then be written as:

$$V_G \frac{dY_i}{dZ} + Y_i \frac{dV_G}{dZ} = -k_{L_i} a C_L A \left( \frac{Y_i}{K_i} - X_{b_i} \right) \quad (2)$$

The sum of all components from i = 1 to n result in:

$$\sum_{i=1}^n \left[ V_G \frac{dY_i}{dZ} \right] + \sum_{i=1}^n \left[ Y_i \frac{dV_G}{dZ} \right] = \sum_{i=1}^n -k_{L_i} a C_L A \left( \frac{Y_i}{K_i} - X_{b_i} \right) \quad (3)$$

Since:

$$\sum_{i=1}^n \frac{dY_i}{dZ} = 0 \text{ and } \sum_{i=1}^n Y_i = 1$$

Equation 3 simplifies to:

$$\frac{dV_G}{dZ} = -A C_L \sum_{i=1}^n k_{L_i} a \left( \frac{Y_i}{K_i} - X_{b_i} \right) \quad (4)$$

Substitution of Equation 4 into Equation 2 results in:

$$V_G \frac{dY_i}{dZ} - Y_i A C_L \sum_{i=1}^n k_{L_i} a \left( \frac{Y_i}{K_i} - X_{b_i} \right) = -k_{L_i} a C_L A \left( \frac{Y_i}{K_i} - X_{b_i} \right) \quad (5)$$

Equation 5 can be rearranged to obtain:

$$\frac{dY_i}{dZ} = \frac{A Y_i C_L}{V_G} \sum_{i=1}^n k_{L_i} a \left( \frac{Y_i}{K_i} - X_{b_i} \right) - \frac{A C_L}{V_G} k_{L_i} a \left( \frac{Y_i}{K_i} - X_{b_i} \right) \quad (6)$$

APPENDIX E

MAJOR EQUIPMENT SUMMARY

MAJOR EQUIPMENT SUMMARY

ENTRAINED BED REACTOR SYSTEM

Description	Number Req'd.	Size	Design		Material
			Temp., °F/Press., psig		
<u>Reactors</u>					
F-T Reactor	2	13 ft ID x 111 ft T-T w/29,000 ft <sup>2</sup> cooling coils	640/450		C-1/2 Mo w/C-1/2 Mo tubes
<u>Other Vessels</u>					
Catalyst Receivers	2	30 ft OD x 40 ft T-T w/cyclones	640/435		C-1/2 Mo
Catalyst Hoppers	4	15 ft OD x 30 ft 8 in T-T	640/450		C.S.
Quench Towers	2	27 ft OD x 80 ft T-T w/4 sieve trays and 3 pans	430/410		316L S.S.
<u>Heat Exchangers</u>					
Comb. Feed vs. Circ. Oil	2	51,000 ft <sup>2</sup>	410/450-Sh 430/450-T		316L-lined 316 tubes
BFW vs. Circ. Oil	2	47,500 ft <sup>2</sup>	430/450-Sh 335/75-T		316L lined 316 tubes
BFW vs. Quench Vapor	2	27,500 ft <sup>2</sup>	330/450-Sh 285/75-T		316L lined 316 tubes
<u>Pumps</u>					
Circ. Oil to BFW Preheat	2	24,100 GPM - 1750 HP			
Circ. Oil to Comb. Feed Exch.	16	7,050 GPM - 450 HP			
<u>Other</u>					
Structural Steelwork	2	350 tons			
Standpipe	2	50 in ID x 75 ft +2 Slide Valves			
Transfer Line	2	80 in ID x 50 ft			
			640/450		1-1/4 Cr-1/2 Mo
			640/450		1-1/4 Cr-1/2 Mo

APPENDIX E (Continued)

MAJOR EQUIPMENT SUMMARY

TUBE-WALL REACTOR SYSTEM

Description	Number Req'd.	Size	Temp., °F/Press., psig	Design	Material
F-T Reactors	52	16 ft ID x 60 ft T-T 106,300 ft <sup>2</sup> tube S.A.	690/60-Sh 690/450-T	690/60-Sh 690/450-T	C.S.-Sh C-1/2 Mo-T
Dowtherm Receiver	52	10 ft ID x 12 ft 7 in T-T	690/100	690/100	C.S.
Feed/Effluent	4	21,490 ft <sup>2</sup>	630/450-Sh 690/450-T	630/450-Sh 690/450-T	C-1/2 Mo, 304L lined 316-T
Steam Generator	52	3,210 ft <sup>2</sup>	690/60-Sh 540/650-T	690/60-Sh 540/650-T	C.S.
Dowtherm Circ. Pump	52	1030 GPM - 20 HP			

Reactors

Other Vessels

Heat Exchangers

Pumps

APPENDIX E (Continued)

MAJOR EQUIPMENT SUMMARY

SLURRY REACTOR SYSTEM

Description	Number Req'd.	Size	Temp., °F/Press., psig	Design Material
F-T Reactors	18	14 ft ID x 27 ft T-T w/9800 ft <sup>2</sup> cooling coils	580/450	C-1/2 Mo
<u>Reactors</u>				
Catalyst Hopper	1	9 ft ID x 15 ft 9 in T-T	500/450	C.S.
<u>Other Vessels</u>				
<u>Heat Exchangers</u>				
Feed Effluent	18	4530 ft <sup>2</sup>	515/450-Sh 465/450-T	304L lined 316 S.S.
Steam Generator	18	1080 ft <sup>2</sup>	640/650-Sh 580/450-T	C.S. K.C.S.
<u>Pumps</u>				
Oil Circ. Pump	18	2000 GPM - 50 HP		

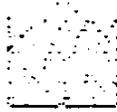
APPENDIX E (Continued)

MAJOR EQUIPMENT SUMMARY

EBULLATING BED REACTOR SYSTEM		Number Req'd.	Size	Temp., °F/Press., psig	Design	Material
Description						
<u>Reactors</u>						
F-T Reactors	20	14 ft ID x 30 ft T-T	600/450		C-1/2 Mo	
<u>Other Vessels</u>						
Vapor/Liquid Separator	20	14 ft ID x 15 ft T-T	600/450		C.S.	
<u>Heat Exchangers</u>						
Feed/Effluent	20	4,740 ft <sup>2</sup>	535/450-Sh		304L lined	
Steam Generator	20	11,750 ft <sup>2</sup>	600/450-T		316	
			640/650-Sh		C.S.	
			600/450-Sh		K.C.C.S.	
<u>Pumps</u>						
Oil Circ. Pump	20	21,800 GPM - 1500 IIP				

APPENDIX F

EBULLATING BED REACTOR DESIGN



# CHEM SYSTEMS INC.

747 Third Avenue, New York, N.Y. (10017)  
Telephone (212) 421-9460 Telex 224649

September 15, 1979

Ms. Mary L. Reikena  
UOP Process Division  
20 UOP Plaza  
Algonquin & Mt. Prospect Roads  
Des Plaines, Illinois 60016

Dear Mary:

Chem Systems is pleased to submit herein two conceptual designs for liquid phase Fischer-Tropsch reactor systems per specifications in your letter of August 7. In the first case a Lurgi-type feed gas is processed, while a K-T type gas is employed in the second design. In both cases it is assumed that the reaction product slates provided by UOP are obtained in a single reactor pass instead of the 1/1 recycle/fresh feed scheme originally proposed by UOP. Two other assumptions that were incorporated into our design are:

- Catalyst volume was determined by employing a space velocity of 300 hr<sup>-1</sup> for the once-through cases. This is one-half of the space velocity originally proposed for the recycle case.
- Circulating oil composition is the same for both cases and equivalent to the resulting equilibrium liquid obtained by flashing the K-T case product slate at the reactor conditions.

There are also two process options that are open to UOP's discretion. They are:

- Temperature of boiler feedwater charged to the oil cooler. This will ultimately set the quantity of 500 psig steam generation.
- The cooling medium(s) and flowscheme to be employed in the final cooling of the product gas stream.

The attached package includes process flow scheme, material balance, reactor effluent vapor cooling curve and major equipment descriptions for each of the two cases examined. Hopefully, the information provided here is in sufficient detail to enable preliminary review of the process, and also enable UOP to determine the proper way to cool the reactor effluent gases. Although a detailed analysis of gas recycle arrangements were not performed, a table

has been included that shows speculative process modifications that would be required to process the two feed gases in this manner. Interestingly enough, the same reactor could be employed for both feed gases whether operating in the once through mode or with recycle gas, namely 14' ID x 70' T-T. Also included is a possible flowscheme for catalyst reduction.

During the development of the two designs, communication between Chem Systems and UOP was quite helpful in arriving at the final flowschemes. Development of these final flowschemes is briefly described below.

Our development of the processes began with the Lurgi feed gas employing a once-through arrangement and assuming that the product slate of the recycle case could be obtained. When this product slate was flashed at the reactor exit conditions no liquid material resulted. In fact, computer results showed the gas stream to be superheated by 210°F. To insure that reactor product vapors would be at their dew point, and an equilibrium liquid (which would be used as circulating liquid) did exist, initially it was assumed that a portion of the liquid product stream was required as recycle back to the reactor. This situation would force more oil into the reactor vapor product until the dew point temperature was increased to 510°F. Under these conditions the oil cooler duty was only 25.0 instead of the 43.3 MM Btu/hr attained in the ultimate design. This represents a substantial reduction in the quantity of reaction heat that could be recovered at high temperature levels in the oil cooler and shifted a large portion of the reaction heat into the gas cooling train. Of course, increasing the reactor pressure would increase the vapor dew point temperature until it was 510°F. Although this would leave the bulk of reaction heat recovery in the oil cooler, the required operating pressure would be above the 500 psig design constraint given. Combinations of increased operating pressure with smaller recycle quantities of liquid product were envisioned but were not felt to be warranted since UOP assured that the reaction product would produce an equilibrium liquid.

Apparently, the actual breakdown of the reaction products contains some materials quite heavier than the average properties provided for the 750+ product cut. These are the materials that UOP has assured will not flash, and they also provided an equilibrium composition for circulating liquid. Production of this stream is extremely small. A review of this composition poses a new problem; is this material suitable as the circulating liquid? The liquid phase reaction system requires a seal flush return for pump seals and wear rings that would ultimately be returned to the circulating liquid. Although the required quantity of this stream is very small, (probably a small portion of the liquid product from the separator) it is much larger than the quantity of flash liquid produced and therefore the circulating would be much lighter than assumed. Thus, the circulating oil composition for the Lurgi case was assumed to be the same as for the K-T case.

Included below are some general comments in regard to the reaction catalyst. First, it may be necessary to install a sulfur guard chamber depending upon the resistance of the catalyst and the sulfur content of the feed gas. This unit could be put after the feed/effluent exchanger and may require an additional heater to attain an adequate temperature for the sulfur guard system. Gas temperature into the Fischer-Tropsch reactor is not that critical since the small sensible heat requirement for the feed gas required for heating or cooling this gas can easily be absorbed by the large bulk of circulating liquid. Feed/effluent exchanger surface could also be decreased if feed gas preheat is reduced below 470°F, without a noticeable change in the reactor system. This can be easily evaluated with the help of the enclosed reactor effluent cooling curves.

Also, a catalyst reduction system will be required and will need ample supply of hydrogen and nitrogen. The system will require as a minimum a feed/effluent exchanger and an additional heater to reach reduction temperatures. If large quantities of reduction gases are required it may be necessary to add a recycle compressor and cooler to insure adequate recycle of the reduction gas and also that this material is sufficiently dry enough for reuse. A typical scheme appears in Figure 5. The catalyst reduction will normally be started before oil circulation is initiated because reduction will take more time than system heat-up. After the reactor is isolated from the main circulating oil supply, process feed gas supply, and main reactor discharge lines, reactor heat-up can begin with nitrogen. Once a suitable temperature is reached (about 400°F), hydrogen flow is begun and nitrogen is shut off. The temperature is gradually increased to reduction temperature and maintained for the reduction period. Catalyst vendors will specify the hydrogen flow rates, reduction temperature and duration. The reduction is usually carried out at atmospheric pressure. At the end of the reduction period, nitrogen flow replaces the hydrogen, and the system temperature is lowered to reaction temperature. The catalyst is now reduced and ready for use. Simultaneously, the circulating oil system must be started up so that the system can be pressurized and the reaction started.

Depending upon the characteristics of the catalyst and the ultimate operation of the process, it may be necessary to install filters on the circulating oil to remove attrited catalyst.

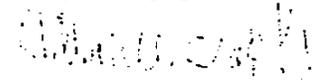
The use of smaller catalyst particles was reviewed and found that they may not be economically justified for this system. By halving the catalyst particle diameter, to 1/32", the catalyst activity was assumed to increase fourfold; simply in direct proportion to surface area. Although this dramatically reduces the catalyst requirement, oil circulation, and possibly reactor diameter, the circulating oil  $\Delta T$  and gas expansion in the reactor become too large.

Ms. Mary L. Reikena  
September 15, 1979  
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CHEM SYSTEMS II

We appreciated this opportunity to provide assistance to UOP as part of its support services contract to DOE. I hope sufficient information has been provided to carefully analyze the designs. Please do not hesitate to contact Marshall or myself should any additional information be required.

Very truly yours,

  
William A. Brophy  
Process Technologist

WAB:mem

cc: MEF, RLM

Table of Inclosures

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FIGURE I - CASE I PROCESS FLOW SCHEME

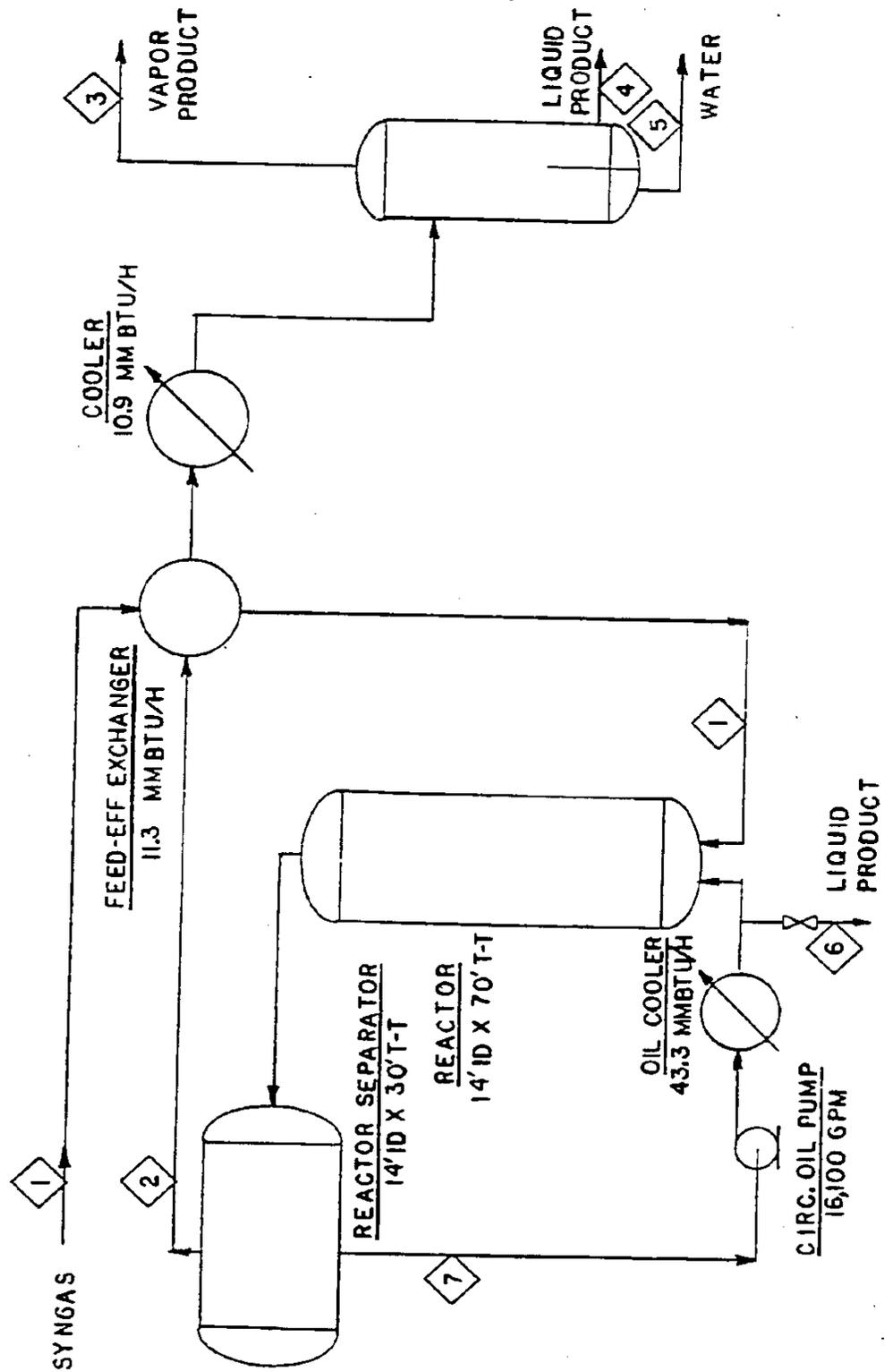


TABLE 1

Case I -- Lurgi Feed Gas - Once-Through-Material Balance (In Lb Mol/Hr)

Component	Mol. Wt.	1 Fresh Feed	2 Reactor Vapor	3 Vapor Product	4 Liquid Product	5 Water Product	6 Heavy Liq. Prod.	7 Reactor Liquid
Hydrogen	2.016	2,262.9	779.8	779.5	0.3			31.6
Carbon Monoxide	28.011	1,132.0	116.4	116.3	0.1			136.9
Carbon Dioxide	44.100	126.3	332.0	330.9	1.1			1,085.1
Methane	16.043	678.5	722.5	721.1	1.4			24.1
Ethylene	28.054		18.5	18.4	0.1			15.0
Ethane	30.070		20.0	19.8	0.2			18.8
Propylene	42.081		22.8	22.3	0.5			35.3
Propane	44.097		6.1	6.0	0.1			9.7
Butylene	56.108		18.2	17.1	1.1			48.9
Butane	58.124		3.5	3.3	0.2			9.7
C5-375°F	98.7		56.36	28.52	27.84			637.6
375-750°F	209.8		8.53	0.01	8.52			3,350.0
750°F+	362.0		0.14	-	0.14			13,325.3
Water	18.016		593.9	11.9	0.1	581.9		287.2
Total, MPH		4,199.7	2,698.73	2,075.13	41.70	581.9	negligible	19,015.2

FIGURE 2 - CASE II PROCESS FLOW SCHEME

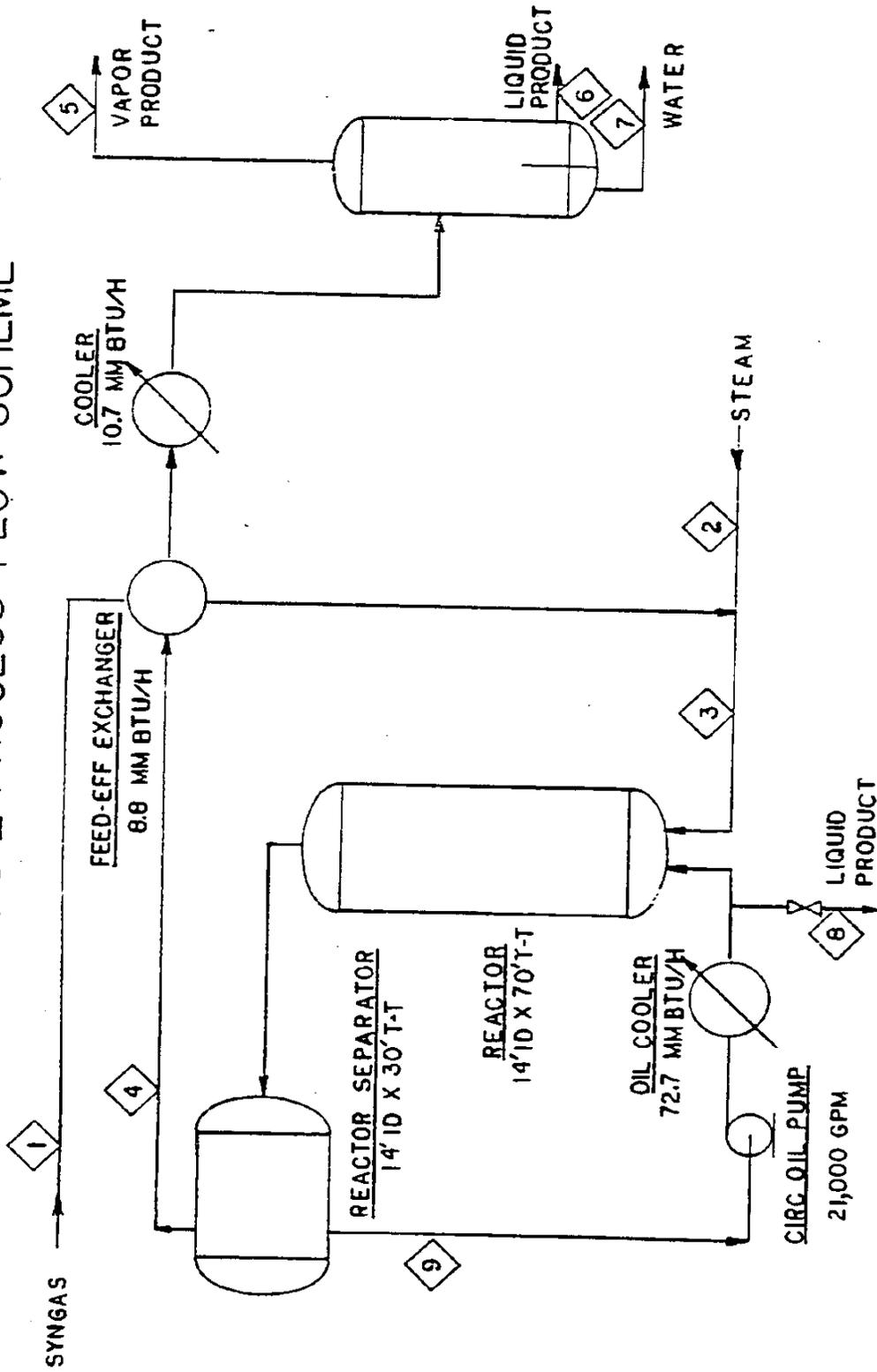


TABLE 2

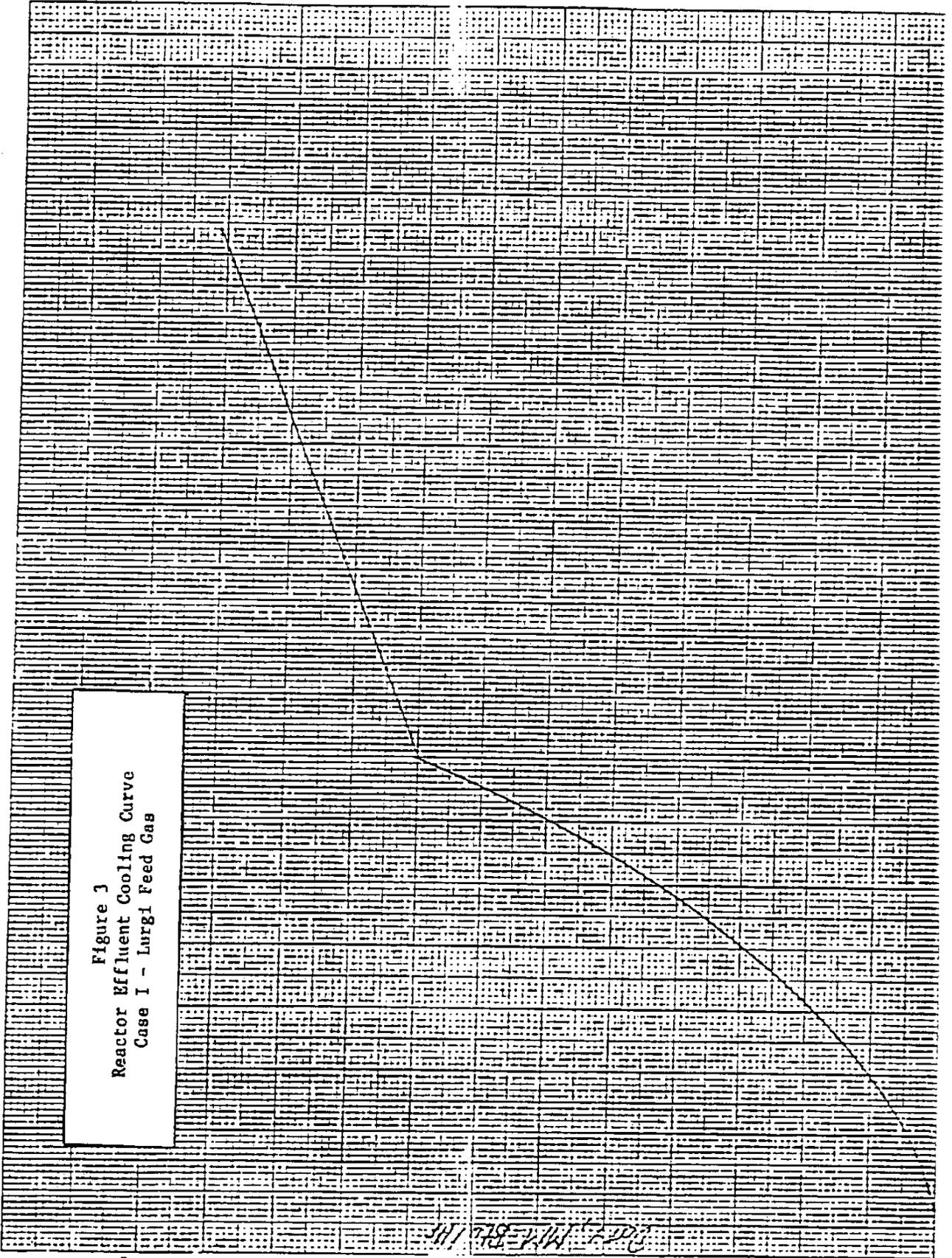
Case 11 -- K-T Feed Gas - Once-Through-Material Balance (In Lb Mol/lir)

Component	Mol. Wt.	1 Fresh Feed	2 Steam Addition	3 Combined Feed	4 Reactor Vapor	5 Vapor Product	6 Liquid Product	7 Water Product	8 Heavy Liq. Prod.	9 Reactor Liquid
Hydrogen	2.016	1,319.7		1,319.7	47.7	47.6	0.1			40.8
Carbon Monoxide	28.011	2,075.1		2,075.1	207.5	207.0	0.5			177.0
Carbon Dioxide	44.100	105.4		105.4	918.5	908.2	10.3		0.1	1,403.1
Methane	16.043				23.2	23.0	0.2			31.1
Ethylene	28.054				9.5	9.3	0.2			19.4
Ethane	30.070				10.3	10.0	0.3			24.3
Propylene	42.081				13.5	12.6	0.9			45.7
Propane	44.097				3.6	3.3	0.3			12.6
Butylene	56.108				12.3	10.2	2.1			63.2
Butane	58.124				2.3	1.9	0.4			12.6
C5-375°F	105.44				57.7	14.7	43.0		0.1	824.5
375-750°F	225.92				24.9		24.9		0.4	4,331.7
750°F+	362.0				1.6		1.6		1.8	17,230.4
Water	18.016		350.0	350.0	530.8	7.2	0.2	523.4		371.4
Total, MPH		3,500.2	350.0	3,850.2	1,863.4	1,255.0	85.0	523.4	2.4	24,587.8

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Figure 3  
Reactor Effluent Cooling Curve  
Case I - Lurgi Feed Gas



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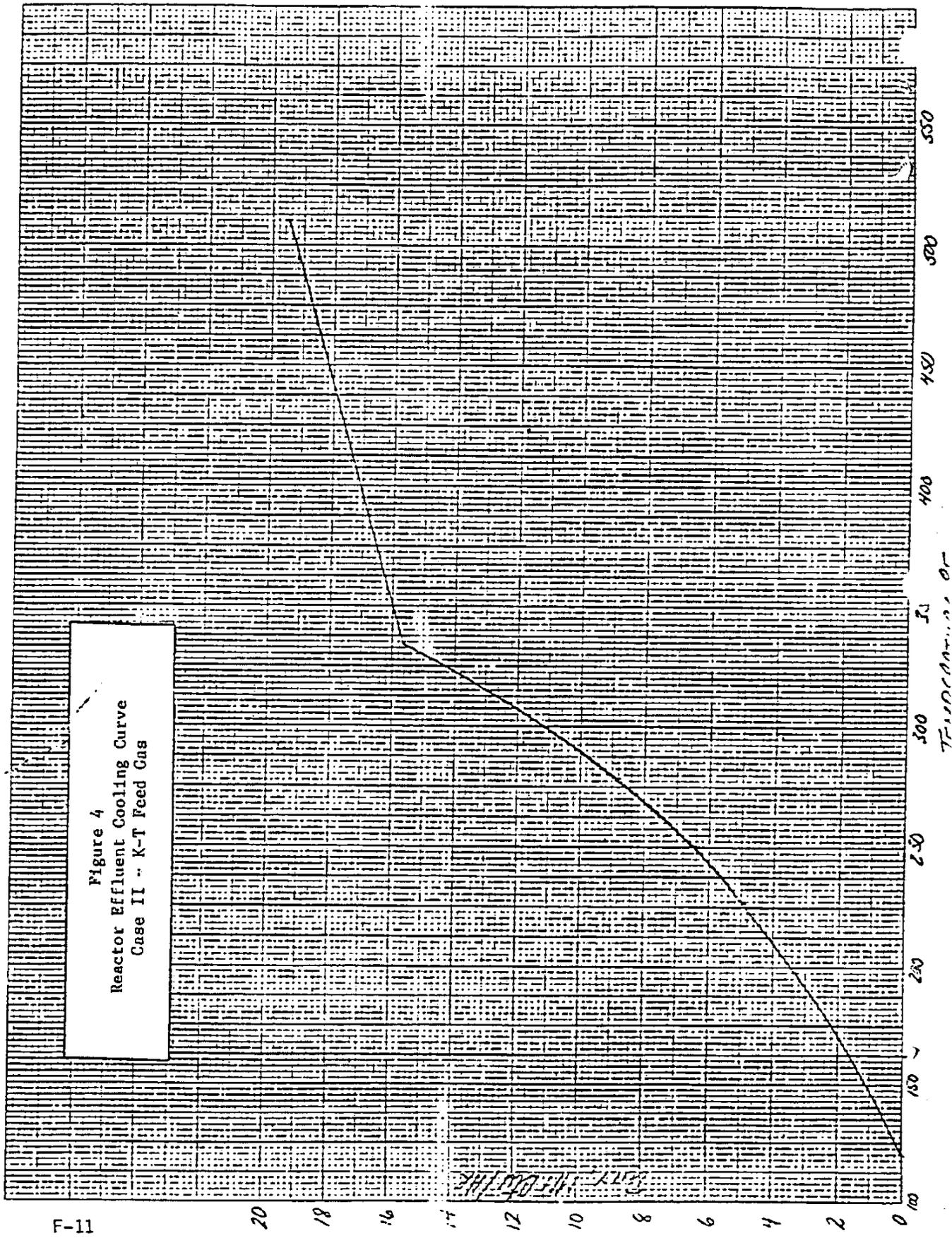


Figure 4  
 Reactor Effluent Cooling Curve  
 Case II - K-T Feed Gas

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TEMPERATURE OF REACTOR EFFLUENT

TIME

Table - 3  
Major Equipment Description

<u>Item</u>	<u>Case I</u> <u>Lurgi Feed Gas</u>	<u>Case II</u> <u>K-T Feed Gas</u>
<u>Reactor</u>		
Dimensions	14' ID x 70' T-T	14' ID x 70' T-T
VHSV, hr <sup>-1</sup>	300	300
Catalyst Size	1/16" Spheres	1/16" Spheres
Catalyst Volume, ft <sup>3</sup>	5,305	4,864
Design Pressure and Temperature	350 psig @ 600°F	
<u>Oil Cooler</u>		
Duty, MM Btu/hr	43.3	72.7
Oil Temp In/Out, °F	510/499	510/496
Steam Generation Pressure	500 psig (470°F)	500 psig (470°F)
Design Pressure Oil/Steam Side	350/550 psig	350/550 psig
Design Temperature Oil/Steam Side	600/525°F	600/525°F
<u>Circulating Oil Pump</u>		
Quantity	1 + spare	1 + spare
Horsepower	750	1,000
Head	50 psi	50 psi
Flowrate, GPM	16,100	21,000
	(17,700) Design	(23,000) Design
<u>Reactor Separator</u>		
Dimensions	14' ID x 30' T-T	
Design Pressure and Temperature	350 psig @ 600°F	
<u>Feed/Effluent Exchanger</u>		
Duty, MM Btu/Hr	11.3	8.8
Reactor Effluent Temp In/Out, °F	510/268	510/296
Cooling Curve, Figure #	3	4
Feed Gas Temp In/Out, °F	120/470	120/470
Design Pressure and Temperature	350 psig @ 600°F	
<u>Final Cooler(s)</u>		
Duty, MM Btu/hr	10.9	10.7
Reactor Effluent Temperature	268/120°F	296/120°F
In/Out, °F		
Cooling Curve, Figure #	3	4
Cooling Medium	BFW and/or CW	
<u>V/L Separator</u>		
Dimensions	4.5' ID x 12' T-T	
Design Pressure and Temperature	350 psig @ 150°F	

Table 4  
Major Process Parameters Changes  
 (Speculative 1/1 Feed/Recycle Gas Case)

	<u>Case I</u> <u>Lurgi Feed Gas</u>	<u>Case II</u> <u>K-T Feed Gas</u>
VHSV, hr <sup>-1</sup>	600	600
Oil Cooler Duty, MM Btu/hr	42.1	71.6
Oil $\Delta T$ , °F	10.7	13.8
Effluent Gas Cooling MM Btu/hr (510°F → 120°F)	33.7	37.0
Feed Gas Heating, MM Btu/hr (120 → 470°F)	11.3	8.8
Recycle Gas Heating, MM Btu/hr (120 → 470°F)	11.3	8.8
Recycle Compressor, HP (260 → 320 psig)	540.0	450.0
Steam Addition, Lbs/Hr		12,611