CHAPTER 5

CONCLUSIONS

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The aims of the present work are modeling and simulation of Fischer-Tropsch slurry bubble column reactor as well as energy conservation in the FT process. The two- class bubble model of **Van der Lann et al. (1999)** was chosen for simulation. The model equations were solved analytically. An overall executive program that calls different subroutines at request to calculate the hydrodynamic and kinetic parameters and at the same time performs the necessary calculations needed for model solution was developed

The developed software was used to reproduce the performance study of an industrial scale slurry F-T bubble column reactor that uses iron based catalyst which was undertaken by **Van der Laan et al. (1999).**

The operating conditions were varied so as to study the effect of superficial gas velocity, solids holdup and H_2/ CO feed ratio on synthesis gas conversion and reactor productivity. It was found that synthesis gas conversion decreases with increasing superficial gas velocity, decreasing solids holdup and decreasing H_2/ CO feed ratio. On the other hand reactor productivity increases with increasing all three variables.

The Software results are similar to those obtained by **Van der Laan et al. [1999].** This confirmed the validity of the proposed method of solution

The same model but with cobalt catalyst based kinetics was used to simulate the performance of the pilot scale slurry reactor of the **FT AFDU** demonstration plant at **Laporte Texas USA.** Simulation studies were performed under different operating conditions.

Conversion of both hydrogen and carbon monoxide are slightly higher than the pilot results. The reason of this discrepancy is thought to be due to diffusivity values necessary to calculate mass transfer coefficients. Diffusivity and hence mass transfer coefficients have strong influence on the reactants concentrations in the bubble column slurry reactor and hence synthesis gas conversion

The parameters of the **ORPDM** of **Van der Laan et al. (1999)** were modified so as to suit selectivity obtained from cobalt catalyst. The model results are in excellent agreement with the reported experimental results for gas holdup and reactor productivity and in fair agreement with the reported conversion and selectivity for light hydrocarbons.

Energy conservation in the pilot scale slurry-phase **FT AFDU** demonstration plant at **Laporte Texas USA** has been attempted in this work. The transshipment model for minimum energy utilization developed at the Egyptian Petroleum Research Institute has been utilized together with LINDO linear programming solver to establish minimum energy utilization.

Five assigned minimum temperature differences, ΔT_{min} namely; 10, 20, 30, 40 and 50 °C were utilized. The results indicated that hot utility was not needed until ΔT_{min} = 30 °C. Thus a total saving of the hot utility was possible. The minimum cost heat exchanger network was chosen among the designed networks at different minimum temperature differences. That corresponded to, ΔT_{min} = 10 °C showed the minimum annualized cost.

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APPENDIX

Appendix: A

Solution of large bubble class differential mass balance equation (2-12)

The large bubble class differential mass balance was represented by Eq. (2-12)

$$\frac{-d\, y_{i,G}^{large}}{dZ} = \frac{(y_{i,G0} + \alpha\, y_{i,G}^{large})^2 (k_L a)_i^{large}\, R\, T\, L}{U_{LB0} (y_{i,G0})^2 (1+\alpha)\, P} \left[\frac{P\, y_{i,G}^{large}}{m_i^{'}} - C_{i,L} \right] \qquad \text{(A-1)}$$

let

$$a = \frac{(k_L a)_i^{large}\, R\, T\, L\, C_{i,L}}{U_{LB0} (y_{i,G0})^2 (1+\alpha)\, P}$$

$$b = \frac{(k_L a)_i^{large} R\, T\, L}{U_{LB0} (y_{i,G0})^2 (1+\alpha)\, m_i^{'}}$$

$$\frac{d(y_{i,G}^{large})}{dZ} = a(y_{i,G0} + \alpha\, y_{i,G}^{large})^2 - b(y_{i,G0} + \alpha\, y_{i,G}^{large})^2\, y_{i,G}^{large} \qquad \text{(A-2)}$$

$$\frac{d(y_{i,G}^{large})}{dZ} = (y_{i,G0} + \alpha\, y_{i,G}^{large})^2\, (a - b\, y_{i,G}^{large}) \qquad \text{(A-3)}$$

$$dZ = \frac{d\,(y_{i,G}^{large})}{(y_{i,G0} + \alpha\, y_{i,G}^{large})^2\, (a - b\, y_{i,G}^{large})} \qquad \text{(A-4)}$$

Analyzing the term $\dfrac{1}{(y_{i,G0} + \alpha\, y_{i,G}^{large})^2\, (a - b\, y_{i,G}^{large})}$

Then

$$\frac{1}{(y_{i,G0}+\alpha\, y_{i,G}^{large})^2(a-b\, y_{i,G}^{large})}$$

$$= \frac{\overline{A}}{(y_{i,G0}+\alpha\, y_{i,G}^{large})^2} + \frac{\overline{B}}{(y_{i,G0}+\alpha\, y_{i,G}^{large})} + \frac{\overline{C}}{(a-b\, y_{i,G}^{large})} \qquad \text{(A-5)}$$

$$= \frac{\overline{A}\,(a-b\, y_{i,G}^{large}) + \overline{B}(y_{i,G0}+\alpha\, y_{i,G}^{large})(a-b\, y_{i,G}^{large}) + \overline{C}(y_{i,G0}+\alpha\, y_{i,G}^{large})^2}{(y_{i,G0}+\alpha\, y_{i,G}^{large})^2(a-b\, y_{i,G}^{large})} \qquad \text{(A-6)}$$

Find the constants $\overline{A}$, $\overline{B}$ *and* $\overline{C}$

$$\overline{A}\,a - \overline{A}\,b\, y_{i,G}^{large} + \overline{B}\,a\, y_{i,G0} + \overline{B}\,a\,\alpha\, y_{i,G}^{large} - \overline{B}\,b\, y_{i,G0}\, y_{i,G}^{large} - \overline{B}\,\alpha\, b\,(y_{i,G}^{large})^2$$

$$+\overline{C}\, y_{i,G0}^2 + 2\,\overline{C}\,\alpha\, y_{i,G0}\, y_{i,G}^{large} + \overline{C}\,\alpha^2\,(y_{i,G}^{large})^2 = 1 \qquad \text{(A-7)}$$

Then

$$\overline{A}\,a + \overline{B}\,a\, y_{i,G0} + \overline{C}\, y_{i,G0}^2 = 1 \qquad \text{(A-8)}$$

$$-\overline{A}\,b - \overline{B}\,b\, y_{i,G0} + \overline{B}\,a\,\alpha + 2\,\overline{C}\,\alpha\, y_{i,G0} = 0 \qquad \text{(A-9)}$$

$$-\overline{B}\,\alpha\, b + \overline{C}\,\alpha^2 = 0 \qquad \text{(A-10)}$$

Then

$$\overline{C} = \overline{B}\,\frac{b}{\alpha} \qquad \text{(A-11)}$$

By substitution of equation (A-11) in equation (A-9)

$$-\overline{A}\,b - \overline{B}\,b\, y_{i,G0} + \overline{B}\,a\,\alpha + 2\,\overline{B}\,\frac{b}{\alpha}\,\alpha\, y_{i,G0} = 0 \qquad \text{(A-12)}$$

$$-\overline{A}\,b + \overline{B}\,b\, y_{i,G0} + \overline{B}\,a\,\alpha = 0 \qquad \text{(A-13)}$$

$$\overline{A}\,b = -\overline{B}\,b\,y_{i,G0} + \overline{B}\,a\,\alpha \tag{A-14}$$

$$\overline{A} = \frac{\overline{B}\left[b\,y_{i,G0} + a\,\alpha\right]}{b} \tag{A-15}$$

By substitution of equation (A-11) and equation (A-15) in equation (A-8)

$$\frac{\overline{B}\left[b\,y_{i,G0} + a\,\alpha\right]}{b}\,a + \overline{B}\,a\,y_{i,G0} + \overline{B}\,\frac{b}{\alpha}\,y_{i,G0}^{2} = 1 \tag{A-16}$$

$$\overline{B}\left[\frac{a}{b}\left[b\,y_{i,G0} + a\,\alpha\right] + a\,y_{i,G0} + \frac{b}{\alpha}\,y_{i,G0}^{2}\right] = 1 \tag{A-17}$$

$$\overline{B} = \frac{1}{\left[\frac{a}{b}\left[b\,y_{i,G0} + a\,\alpha\right]\right] + a\,y_{i,G0} + \frac{b}{\alpha}\,y_{i,G0}^{2}} \tag{A-18}$$

$$\int_{0}^{1} dZ = \left[\frac{-\overline{A}}{\alpha\,(y_{i,G0} + \alpha\,y_{i,G}^{large})} + \frac{\overline{B}}{\alpha}\ln(y_{i,G0} + \alpha\,y_{i,G}^{large}) + -\frac{\overline{C}}{b}\ln(a - b\,y_{i,G}^{large})\right]_{0}^{1} \tag{A-19}$$

$$\left[\frac{-\overline{A}}{\alpha\,(y_{i,G0} + \alpha\,y_{i,G}^{large})}\right] = \frac{\overline{A}}{\alpha\,(y_{i,G0})(1+\alpha)} + \frac{-\overline{A}}{\alpha\,(y_{i,G0} + \alpha\,y_{i,G}^{large})} \tag{A-20}$$

$$= \frac{-\overline{A}(1+\alpha)\ (y_{i,G0}) + \overline{A}(y_{i,G0} + \alpha\, y_{i,G}^{large})}{\alpha\,(y_{i,G0})(1+\alpha)\,(y_{i,G0} + \alpha\, y_{i,G}^{large})} \qquad \text{(A-21)}$$

$$= \frac{-\overline{A}\ (y_{i,G0}) - \overline{A}\ (y_{i,G0})\alpha + \overline{A}\ (y_{i,G0}) + \alpha\,\overline{A}(y_{i,G}^{large})}{\alpha\,(y_{i,G0})(1+\alpha)\,(y_{i,G0} + \alpha\, y_{i,G}^{large})} \qquad \text{(A-22)}$$

$$= \frac{-\overline{A}\,\alpha\ \ (y_{i,G0} - y_{i,G}^{large})}{\alpha\,(y_{i,G0})(1+\alpha)\,(y_{i,G0} + \alpha\, y_{i,G}^{large})} \qquad \text{(A-23)}$$

$$= \frac{-\overline{A}\ \ (y_{i,G0} - y_{i,G}^{large})}{(y_{i,G0})(1+\alpha)\,(y_{i,G0} + \alpha\, y_{i,G}^{large})} \qquad \text{(A-24)}$$

$$\left[\frac{\overline{B}}{\alpha}\ln(y_{i,G0} + \alpha\, y_{i,G}^{large})\right]_0^1 = \frac{\overline{B}}{\alpha}\ln(y_{i,G0} + \alpha\, y_{i,G}^{large}) - \frac{\overline{B}}{\alpha}\ln(1+\alpha)y_{i,G0}$$

$$= \frac{\overline{B}}{\alpha}\ln\frac{(y_{i,G0} + \alpha\, y_{i,G}^{large})}{(1+\alpha)y_{i,G0}} \qquad \text{(A-25)}$$

$$\left[-\frac{\overline{C}}{b}\ \ln(a - b\, y_{i,G}^{large})\right]_0^1 = -\frac{\overline{C}}{b}\ln(a - b\, y_{i,G}^{large}) + \frac{\overline{C}}{b}\ln(a - b\, y_{i,G0})$$

$$= \frac{\overline{C}}{b}\ln\frac{(a - b\, y_{i,G0})}{(a - b\, y_{i,G}^{large})} \qquad \text{(A-26)}$$

Finally equation (A-1) becomes:

$$Z = \frac{-\overline{A}\ \ (y_{i,G0} - y_{i,G}^{large})}{(y_{i,G0})(1+\alpha)\,(y_{i,G0} + \alpha\, y_{i,G}^{large})} + \frac{\overline{B}}{\alpha}\ln\frac{(y_{i,G0} + \alpha\, y_{i,G}^{large})}{(1+\alpha)y_{i,G0}} + \frac{\overline{C}}{b}\ln\frac{(a - b\, y_{i,G0})}{(a - b\, y_{i,G}^{large})} \qquad \text{(A-27)}$$

```
DECLARE SUB TIME ()
DECLARE SUB READATA ()
DECLARE SUB CARBONUM ()
DECLARE SUB HENER ()
DECLARE SUB ALFA ()
DECLARE SUB HeatCof ()
DECLARE SUB EngBL ()
DECLARE SUB RNX ()
DECLARE SUB PhyProp ()
DECLARE SUB HydPra ()
DECLARE SUB Results ()
DECLARE SUB SaveData ()
DECLARE SUB PrintData ()
DECLARE SUB READDATA ()
DECLARE SUB InputData ()
```

'*** MODEL CALCULATIONS ***

```
 DIM SHARED TR, TR$, TRI, TRI$, TC, TC$, P, P$, L, L$, D1, D1$, DHR, DHR$
 DIM SHARED RG, RG$, RGO, RGO$, ES, ES$, CF, CF$, UO, UO$, UG, UG$, G$, UGO$
 DIM SHARED US, US$, RL, RL$, VL$, TCL$, EDO$, CpL$, DLO$, TCC$, CpC$,G, XI(50)
 DIM SHARED VL, TCL, EDO, CpL, DLO, TCC, CpC, RP, RP$, RSK, RSK$, NC, UGO
 DIM SHARED YS(50), YL(50), YSI(50), ya(50), YO(50), C$(10), HC(50), LRT
 DIM SHARED DL(50), VD, EDF, UDF, ULB, EL, EG, RX, KLaL(40), KLaS(40), KC2
 DIM SHARED Z(150), Z1(20), Z2(20), Z3(20), KA, RSL, DR(20), CpS, HE, F(20)
 DIM SHARED V, adb(50), ED, edd, RFT, TCS, VS, ACC, RT(30), X1E, X2E, R$
 DIM SHARED AC1(10), B(150), K, m, Q, SUM, DTitle$, HE1, UG1, ZI(100), MTOP(50)
 DIM SHARED Tcat, CC(150), BC(150), AC(120), R, CLM1(10), CLM2(10), CLM3(10)
 DIM SHARED DT$, DM$, CL1(10), CL2(10), CL3(10), CLM(50), DFileName$, ZO(50)
 DIM SHARED MO(50), MP(50), WO(50), WP(50), WW1(50), MWT(20), WCO(50), WCP(50)
 DIM SHARED XA(10), ELB, NC$, YLI(100), IT, YLO(50), A(150), KK, YG(20), KCO
 DIM SHARED MC1, MC2P, MC2O, KC1, KC24, KC26, XO(60), XP(60), YP(60), KH, KN2
 DIM SHARED INTG(50), SUM(50), X1E(50), X2E(50), Q(50), CL(50), PF1$, N, TT7
 DIM SHARED T0, PP, KR, ALF2, ALF(50), CT1, TP1, TP2, C, MC(50), KC36, KC38,
 DIM SHARED TT1$, TT2, TT2$, TT3, TT4, TT5, TT6, TT1, X1(50), X2(50), Y1(50),
 DIM SHARED MCNP(50), MCNO(50), SUMT, KI(50), FY(50), SUMP, SUMO, SUM1, SUMT2
 DIM SHARED MCOP(50), MC2T, MTOT(50), Y2(50)
  PRINT "DATE  "; DATE$, "TIME  "; TIME$

'CALCULATIONS CONSTANTS
'------------------
  MH$ = "MOL. WEIGHT OF H2;MH(g/mol):"
  MCO$ = "MOL. WEIGHT OF CO;MCO(g/mol):"
  R$ = "GAS CONST.;R(pa.m^3/(mole.k):"
  G$ = "GRAVITY ; G,(m^2/s)"
  R = 8.314: G = 9.8
  PF1$ = "##.####"
  PF5$ = "####.####"
  PRINT " REACTOR CONDITIONS"
  PRINT "_____________________"
  TR$ = "Reactor Temperature  (K):"
  TRI$ = "Inlet Reactor Temperature  ;TRI,(K):"
  TC$ = "Cooling Temperature  ;TC,(K):"
   P$ = "Reactor Pressure  ;P,(pa):"
   L$ = "Reactor Length  ;L,(m):"
   D1$ = "Reactor Length  ;D1,(m):"
   DHR$ = "Reaction Enthalpy  ;DHR,(J/mol):"
   RG$ = "Density of Gas at Reactor Condition ;RG,(kg/m^3):"
   RGO$ = "Density of Gas at Ambient Condition  ;RGO,(kg/m^3):"
```

```
  TR$ = "Reactor Temperature  (K):"
  TRI$ = "Inlet Reactor Temperature  ;TRI,(K):"
  TC$ = "Cooling Temperature  ;TC,(K):"
   P$ = "Reactor Pressure  ;P,(pa):"
   L$ = "Reactor Length  ;L,(m):"
   D1$ = "Reactor Length  ;D1,(m):"
   DHR$ = "Reaction Enthalpy  ;DHR,(J/mol):"
   RG$ = "Density of Gas at Reactor Condition ;RG,(kg/m^3):"
   RGO$ = "Density of Gas at Ambient Condition  ;RGO,(kg/m^3):"
   ES$ = "Slurry Hold up  ;ES,(m^3l/m^3r):"
   CF$ = "Contraction Factor   ;CF:"
   UO$ = "Rise Vel. of the Small Bubbles at 0 Solids ;UO,(m/s):"
   UG$ = "Inlet Superfacial Velocity  ;UG,(m/s):"
   US$ = "Slurry Velocity  ;US,(m/s):"
   PRINT " LIQUID PROPERTIES"
   RL$ = "Liquid Density  ;RL,(kg/m^3):"
   VL$ = "Liquid Viscosity  ;VL,(pa-s):"
   TCL$ = "Thermal Conductivity of Liquid   ;TCL,(w/m.K):"
   EDO$ = "Refrence Hold up at Pure Liquid  ;EDO:"
   CpL$ = "Heat Capacity of Liquid   ;CpL,(j/kg.K)):"
   DLO$ = "Diffusivity at Reference Condition  ;DLO,(m^2/s):"
   PRINT "CATALYST PROPERTIES"
   TCC$ = "Thermal Conductivity of Catalyst   ;TCC,(w/m.K):"
   CpC$ = "Heat Capacity of Catalyst  ;CpC,( j/(kg.K)):"
   RP$ = "Catalyst Particle Density  ;RP,(kg/m^3):"
   RSK$ = "Skelton Density  ;RSK,(kg/m^3):"
   PRINT "FEED PROPERTIES"
   NC$ = "No of Component   ;NC:"
   'READ &PRINT DATA
'------------------
INPUT "Enter 1 if you want to read the data from the keyboard &2 from disk
file;DIN:", DIN
SELECT CASE DIN
CASE 1:
      CALL InputData
CASE 2:
      CALL READDATA
  END SELECT
  CALL Results
CLS

    INPUT "Enter -1 if you want to perform the calcn &0 if not ;CAL", CAL
    OPEN "D:LMK.bas" FOR OUTPUT AS #1
    PRINT #1, "DATE  "; DATE$, "TIME  "; TIME$
    PRINT #1, TAB(25); "*** INPUT DATA PRINT OUT ***"
    PRINT #1, TAB(23); "================================"
    PRINT #1, "REACTOR CONDITIONS"
    PRINT #1, "Reactor Temperature  ;TR,(K)="; TR
    PRINT #1, "Reactor Inlet Temperature  ;TRI,(K):", TRI
    PRINT #1, "Reaction Enthalpy  ;DHR,(J/mol)="; DHR
    PRINT #1, "Reactor Length  ;L,(m)="; L
    PRINT #1, "Reactor Diameter  ;D,(m)="; D1
    PRINT #1, "Reactor Pressure  ;P,(pa)="; P
    PRINT #1, "Inlet Superfacial Velocity  ;UG,(m/s)="; UG
    PRINT #1, "Density of Gas at Reactor Condition  ;RG,(kg/m^3)="; RG
    PRINT #1, "Density of Gas at Ambient Condition ;RGO,(kg/m^3)="; RGO
    PRINT #1, "Slurry Hold up  ;ES,(m^3l/m^3r)=:"; ES
    PRINT #1, "Rise Vel. of the Small Bubbles at 0 Solids  ;UO,(m/s =:"; U
    PRINT #1, "Cooling Temperature  ;TC,(K)=:"; TC
```

```
    PRINT #1, "Slurry Velocity  ;US,(m/s)=:"; US
    PRINT #1, "Diffusivity at Reference Condition  ;DLO,(m^2/s)=:"; DLO
    PRINT #1, "Gravity  ;G,(m/s^2)=:"; G
    PRINT #1,

    PRINT #1, "LIQUID PROPERTIES"
    PRINT #1, "--------------------"
    PRINT #1, "Liquid Density  ;RL,(kg/m^3)="; RL
    PRINT #1, "Refrence Hold up at Pure Liquid  ;EDO=:"; EDO
    PRINT #1, "Liquid Viscosity  ;VL,(m/s)="; VL
    PRINT #1, "Thermal Conductivity of Liquid   ;TCL,()="; TCL
    PRINT #1, "Heat Capacity of Liquid    ;CpL,(j/kg.k))="; CpL
    PRINT #1,
    PRINT #1, "CATALYST PROPERTIES"
    PRINT #1, "-----------------------"
    PRINT #1, "Catalyst Particle Density  ;RP,(kg/m^3) ="; RP
    PRINT #1, "Skelton Density   ;RSK,(kg/m^3)="; RSK
    PRINT #1, "Thermal Conductivity of Catalyst  ; TCC,(w/m.K):="; TCC
    PRINT #1, "Heat Capacity of Catalyst   ;CpC,( j/(kg.k)):="; CpC
    PRINT #1, " FEED PROPERTIES "
    PRINT #1, "---------------------"
    PRINT #1, "Gas Constant  ;R,(pa*m^3/(mol*K))="; R
    PRINT #1, "No of Component  ;NC=:"; NC
    PRINT #1,
FOR I = 1 TO NC
 '---------------
  PRINT #1, "C$("; I; ")="; C$(I)
  PRINT #1, "The Mol.Fr.of "; C$(I); " in the Feed YO("; C$(I); ") = "; YO(I)
  PRINT #1, "Henery Co. for "; C$(I); ", HC("; C$(I); "),(Pa.m^3/mol)="; HC(I)
  PRINT #1, "Diffusivity for DL ("; C$(I); ") , (m ^ 2 / s) = "; DL(I); ""
NEXT I
 '--------
   PRINT #1, TAB(27); "*** RESULTS PRINT OUT ***"
   PRINT #1, TAB(23); "==================================="
  'SUB CALCULATIONS
   '_________________

   CALL HydPra
   CALL PhyProp
   CALL RNX

  ' Calculation the ( ys ,Small Bubble Mole Fraction & Concentration
   '-------------------------------------------------------------------
   LRT = L * R * TR
 FOR I = 1 TO NC
'_____________________
6   CL1(I) = -P * YO(I) * UDF / (LRT * KLaS(I))
    ya(I) = ULB * YO(I) ^ 2 * (1 + CF)
    YS(I) = .16 * YO(I)    'ys mole fr. of component i gas in small bubble
    CL2(I) = (YO(I) - YS(I)) / (YO(I) + CF * YS(I))
    CL3(I) = P * YS(I) / HC(I)


    'CALCULATION OF (CAL)   RELATED WITH  YS=  CL(I)
    '"-----------------------------------------------"
    CL(I) = CL1(I) * CL2(I) + CL3(I)
    PRINT #1, "YS("; C$(I); ")="; YS(I), ";CL1("; C$(I); ")="; CL1(I)
    PRINT #1, "CL2("; C$(I); ")="; CL2(I), ";CL3("; C$(I); ")="; CL3(I)
    PRINT #1, "CL("; C$(I); ")="; CL(I)
  ' Calculation  YL ,mole Fraction of H2 in large bubble&relation with Z"
  '-------------------------------------------------------------------
```

```
  '1 - Calculation of  Z
  '_____________________
    IT = 0
10  A1 = CL(I) * KLaL(I) * LRT                          '"calc. of  a  const"
    a2 = ya(I) * P
    A(I) = A1 / a2
    B1 = LRT * KLaL(I)                                 '"calc. of b const"
    B2 = ya(I) * HC(I)
    B(I) = B1 / B2
    adb(I) = A(I) / B(I)
    BC1(I) = adb(I) * (A(I) * CF + B(I) * YO(I))       '"calc. of BC   Const"
    BC2(I) = B(I) / CF * YO(I) ^ 2
    BC3(I) = A(I) * YO(I)
    BC(I) = 1 / (BC1(I) + BC2(I) + BC3(I))
    CC(I) = BC(I) * B(I) / CF                         '"calc. of CC   Const"
    AC1(I) = A(I) * CF + B(I) * YO(I)                 '" calc. of AC  Const"
    AC(I) = BC(I) * AC1(I) / B(I)
    W = adb(I)
    Q = W + .03
    SUM = 0
    J = 0
  FOR K = Q TO .9999 * YO(I) STEP .0001
'---------------------------
    YL(I) = K
20  Z1N = AC(I) * (YL(I) - YO(I))                              ' Z Calculations
    Z1D = (1 + CF) * YO(I) * (YO(I) + CF * YL(I))
    Z1 = Z1N / Z1D
    Z2N = (YO(I) + CF * YL(I))
    Z2D = ((1 + CF) * YO(I))
    Z2 = BC(I) / CF * LOG(Z2N / Z2D)
    Z3N = (A(I) - B(I) * YO(I))
    Z3D = (A(I) - B(I) * YL(I))
    Z3 = CC(I) / B(I) * LOG(Z3N / Z3D)
    Z(I) = Z1 + Z2 + Z3
    IF YL(I) = Q THEN
    ZO(I) = Z(I)
       IF Z(I) > 1 THEN
       GOTO 35
       ELSE
       GOTO 30
       END IF
     END IF
     IF Z(I) > 1 THEN : GOTO 35
     IF ABS(Z(I) - m) <= .0001 THEN 30
     GOTO 40
30   J = J + 1
     YLI(J) = YL(I)
     ZI(J) = Z(I)
34   SUM = SUM + 2 * YL(I)
35   m = Z(I) - .03
40   IF (Z(I) - m) > 0 THEN 60
50   IF (Z(I) - m) < 0 THEN 70
60   KK = YL(I)
     GOTO 80
70   YL(I) = (KK + YL(I)) / 2:          GOTO 20

80 NEXT K
'------------

  '2  - Calculation of Modefied Liquid Concenteration  ;CLM, (mol/m^3)
'_____________________________________________________________________
```

```
    SUM = SUM - Q - YL(I)
    INTG = (.03 / 2) * SUM
    CLM1(I) = KLaL(I) * P * INTG / HC(I)
    RT(I) = F(I) * RX
    CLM2(I) = KLaS(I) * P * YS(I) / HC(I)
    IF C$(I) = "N2" THEN GOTO 81
    CLM3(I) = (KLaS(I) + KLaL(I) + US / L) + (RT(I) / CL(I))  ''
    GOTO 82
81  CLM3(I) = (KLaS(I) + KLaL(I) + US / L) ''
82  CLM(I) = (CLM1(I) + CLM2(I)) / CLM3(I)                    ''
    AE = CF * P
    BE = P * YO(I) - (HC(I) * (CL1(I) + CF * CLM(I)))
    CE = YO(I) * HC(I) * (CL1(I) - CLM(I))
    SRE = SQR(BE * BE - 4 * AE * CE)
    X1E = (-BE + SRE) / (2 * AE)
    X2E = (-BE - SRE) / (2 * AE)
    YSI(I) = CLM(I) * HC(I) / P                'BY HENERY COEF.
    IF X1E >= YSI(I) AND X1E <= YO(I) THEN YS(I) = X1E
    IF X2E >= YSI(I) AND X2E <= YO(I) THEN YS(I) = X2E
90  IF ABS((CLM(I) - CL(I)) / CLM(I)) <= .0919 THEN 100
    CL(I) = CLM(I)
    IT = IT + 1
    A(IT) = A(I): B(IT) = B(I): adb(IT) = adb(I)
    AC(IT) = AC(I): BC(IT) = BC(I): CC(IT) = CC(I)
    YS(IT) = YS(I): ZO(IT) = ZO(I): YLO(IT) = Q: CLM(IT) = CLM(I)
    YSI(IT) = YSI(I): INTG(IT) = INTG: X1E(IT) = X1E: X2E(IT) = X2E
    SUM(IT) = SUM: Z(IT) = Z(I): YL(IT) = YL(I)
    GOTO 10
100 'PRINT #1,
    PRINT #1, "-----------------------------------------------------------------"
    'PRINT #1,
    'PRINT #1, "NO OF ITERATION="; IT
    PRINT #1,
    PRINT #1, "FOR COMPONENT  OF :"; C$(I)
  FOR TT = 2 TO IT
  '---------------
    PRINT #1, TT; TAB(10); a(TT);
    PRINT #1, TAB(25); USING PF1$; adb(TT);
    PRINT #1, TAB(40); USING PF1$; AC(TT);
    PRINT #1, TAB(55); USING PF1$; BC(TT);
    PRINT #1, TAB(70); USING PF1$; CC(TT)
  NEXT TT
    PRINT #1, "-----------------------------------------------------------------"
    PRINT #1, "IT"; TAB(10); "   INTG"; TAB(25); "  SUM";
    PRINT #1, TAB(40); "   X1E"; TAB(55); "   YS"; TAB(70); "   YSE"
    PRINT #1, "-----------------------------------------------------------------"
  FOR TT = 2 TO IT
  '---------------
    PRINT #1, TT; TAB(10); INTG(TT);
    PRINT #1, TAB(25); USING PF1$; SUM(TT);
    PRINT #1, TAB(40); USING PF1$; X1E(TT);
    PRINT #1, TAB(55); USING PF1$; YS(TT);
    PRINT #1, TAB(70); USING PF1$; YSI(TT)
  NEXT TT
  '---------
    PRINT #1, "-----------------------------------------------------------------"
    PRINT #1, "IT"; TAB(10); "   CLM"; TAB(25); "  ZO";
    PRINT #1, TAB(40); "   YLO"; TAB(55); "   ZI"; TAB(70); "   YLI"
    PRINT #1, "-----------------------------------------------------------------"
```

```
FOR TT = 2 TO IT
'---------------
  PRINT #1, TT; TAB(10); USING PF1$; CLM(TT);
  PRINT #1, TAB(25); USING PF1$; ZO(TT);
  PRINT #1, TAB(40); USING PF1$; YLO(TT);
  PRINT #1, TAB(55); USING PF1$; Z(TT);
  PRINT #1, TAB(70); USING PF1$; YL(TT)
NEXT TT
  PRINT #1, "***************************************"
  PRINT #1, "PROFILE OF GAS OUTLET FROM REACTOR"
  PRINT #1, "L"; TAB(20); "YLP("; C$(I); ")"; TAB(45); "ZP("; C$(I); ")"
  PRINT #1, "-----------------------------------------------------------------"
  PRINT #1,
FOR KL = 1 TO J
'---------------
  IF C$(I) = "N2" THEN YLI(KL) = YO(I)
  PRINT #1, KL; TAB(20); USING PF1$; YLI(KL);
  PRINT #1, TAB(45); USING PF1$; ZI(KL)
NEXT KL
'--------

  'Calculation the Gas Conversion of the Component I
  '_________________________________________________

  ' The Mass Balance of the Gas Phase at the Outlet of the Reactor
  '_____________________________________________________________
  U1 = (ULB * Q * YO(I)) / (YO(I) + CF * Q)
  U2 = (UDF * YS(I) * YO(I)) / (YO(I) + CF * YS(I))
  U3 = U1 + U2
  YG(I) = (U3 * YO(I)) / (UG * YO(I) - (U3 * CF))
  IF C$(I) = "N2" THEN YG(I) = YO(I)
  XA(I) = (YO(I) - YG(I)) / (YO(I) + CF * YG(I))
  UG1 = UG * (1 + CF * XA(I))
  XHC(I) = ((UG1 / UG) - 1) / CF
  RT = R * TR
  UT1 = ((ULB * ELB) + (UDF * EDF)) / (EDF + ELB)
  YT(I) = ((YS(I) * EDF) + (YG(I) * ELB)) / (EDF + ELB): CVT = 150
  PRINT #1, "-----------------------------------------------------------------"
  PRINT #1,"Outlet Mole Fr in the L Gas Bubbles of (; C$(I);")=";YG(I)
  PRINT #1, "Outlet Mole Fr in the S Bubbles of (; C$(I); ")=";YS(I)
  PRINT #1,"Avg.Outlet M.Fr in the (S+L) Gas Bubbles of(";C$(I);")=";YT(I)
  PRINT #1, "The Liquid Phase Concn, (mole/m3) of (; C$(I); ")="; CLM(I)
  PRINT #1,"V Conc.in the L Gas Bubbles,(mole/m3)of(";C$(I);")="; CLM1(I)
  PRINT #1,"V Conc.in the S Gas Bubbles,(mole/m3)of(; C$(I);")=";CL1(I)
  PRINT #1,"The Avg.Vap Phase Conc. in (S+L) Gas Bubbles,(mole/m3) of (;
           C$(I); ")="; CVT(I)
  PRINT #1, "Total Vapor Phase Concn. in the (Small+Large) Gas Bubbles ,
           mole/m3="; CVT
  PRINT #1, "Gas Outlet Velocity from krishna calcn ;UG1(m/s)="; UG1
  PRINT #1,"Gas Outlet Vel. from (Small + Large) Gas Bubbles,(m/s) ="; UT1
  PRINT #1, "Conversion %  ;XA("; C$(I); ")="; XA(I)
NEXT I
  CALL HeatCof
  CALL EngBL
  CALL RNX
  PRINT #1, TAB(17); "***INDIVIDUAL HYDROCARBON PRODUCT FORMATION RATES***"
  PRINT #1, TAB(14);    CALL ALFA
  PI = 3.14
  A1 = D1 ^ 2 * PI / 4
  WC1 = L * A1 * 16 * RX * MC1
  WC21 = L * A1 * 28 * RX * MC2O
```

```
    WC22 = L * A1 * 30 * RX * MC2P
    WC2 = WC12 + WC22
    MTOP = 0: MTO = 0: MTP = 0
  FOR I = 3 TO 50
      MO(I) = I * 12 + I * 2
      MP(I) = I * 12 + I * 2 + 2
      WCO(I) = A1 * L * MO(I) * RX * MCNO(I)
      WCP(I) = A1 * L * MP(I) * RX * MCNP(I)
      MTOP(I) = WCO(I) + WCP(I)
      MTO = MTO + WCO(I)
      MTP = MTP + WCP(I)
      MTOP = MTOP + MTOP(I)
    NEXT I
      TOT = MTOP + WC1 + WC21 + WC22
      WC2 = WC21 + WC22
      MO = MTO + WC21
      MP = MTP + WC22
      SOP = MO + MP

   PRINT #1, "-------------------------------------------------------------------"
   PRINT #1, "COMP"; TAB(10); "WT Ratio "; TAB(23); " Para /Tot "; TAB(35);
             "Olef/ Tot"; TAB(50); "Olef/Para"
   PRINT #1, "-------------------------------------------------------------------"
   PRINT #1, "C(1)"; USING PF5$; TAB(10); WC1 / TOT
   PRINT #1, "C(2)"; USING PF5$; TAB(10); WC2 / TOT; TAB(23); (WC22) / TOT;
             TAB(35); WC21 / TOT; TAB(50); WC21 / WC22
 FOR I = 3 TO N
   PRINT #1, "C("; (I); ")"; USING PF5$; TAB(10); MTOP(I) / TOT; TAB(23);
            WCP(I) / TOT; TAB(35); WCO(I) / TOT; TAB(50); WCO(I) / WCP(I)
 NEXT I
   PRINT #1,"COMP";TAB(14);"MI";TAB(30);"Para selec "; TAB(50);"Olef selc"
   PRINT #1, "-------------------------------------------------------------"
   PRINT #1, "C(1)"; USING PF5$; TAB(10); MC1
   PRINT #1, "C(2)"; USING PF5$; TAB(10); MC2T; TAB(30); MC2P; TAB(50); MC2O
 FOR I = 3 TO N
   PRINT #1, "C("; (I); ")"; USING PF5$; TAB(10); MCOP(I); TAB(30); MCNP(I);
            TAB(50); MCNO(I)
 NEXT I
   PRINT #1, "-------------------------------------------------------------"
   PRINT #1, "Total production rates of hydrocarbons, kg/hr ="; TOT
   PRINT #1, "Oefin /TOT="; MO / SOP
   PRINT #1, "Parafin /TOT="; MP / SOP
   PRINT #1, "-------------------------------------------------------------------"
   PRINT #1,
   TT2$ = TIME$
   PRINT #1, TT1$, TT2$
   CALL TIME
   PRINT #1, "Operating Time="; TT7; "SEC."

  CLOSE #1
 END
'
 ------------

SUB ALFA
     FOR CT1 = .02 TO .125 STEP .0001
       F1 = .4: F2 = .6: P1 = 3 '" PRESSURE MPA" P * 10 ^ -6  'F1,F2 FEED RATIO
       KR = .17:  TP1 = 6.5:   TP2 = 1.7: C = .35: N = 50':CT1 = .10639
       T0 = 3.71 * ((P1 * F1) ^ -.5)                          'T0,PC,KR CONST
       T0 = 5.6
       PP = 14 * ((P1 * F1) ^ -.26) * ((P1 * F2) ^ .4)
       PP = 17.4
```

```
      MC1 = CT1 * TP1 ': KR = 0
      KR2 = 17.6 * KR * EXP(2 * C)                    'Calc of ALF2
      T2 = T0 ^ 2 / (1 + KR2)
      ALF2 = PP / (T2 + TP2 + PP)
      MC2P = TP2 * ALF2 * CT1            'Cal of C2 in Paraffin Molar Selec
      MC2O = ALF2 * CT1 * T2             'Calc. of C2 in Olefin in Molar Selec
      CTN = CT1 * ALF2
      SUM = 0: SUMP = 0
      SUMT1 = 0: SUMT2 = 0
      PRINT #1, "MC1="; MC1
      PRINT #1, "-------------------------------------------------------------"
      PRINT #1, "N"; TAB(10); "MCNP(N)"; TAB(20); "SUMP"; TAB(30); "SUMP1";
                TAB(40); "MCNO(I)"; TAB(50); "SUMO"; TAB(60); "SUMO1"
      PRINT #1, "-------------------------------------------------------------"
      PRINT #1,

    FOR I = 3 TO N
    '---------------
      T3 = T0 / (1 + KR * EXP(I * C))
      ALF(I) = PP / (T3 + 1 + PP)
      CTN = CTN * ALF(I)
      MCNP(I) = CTN                     'Calc. of Paraffin in Molar Selec
      MCNO(I) = MCNP(I) * T3                'Calc. of Olefin in Molar Selec
      SUMP = SUMP + MCNP(I)
      SUMP1 = SUMP1 + MCNP(I) * I
      SUMO = SUMO + MCNO(I)
      SUMO1 = SUMO1 + MCNO(I) * I
      SUMT = SUMO1 + SUMP1
      MCOP(I) = MCNP(I) + MCNO(I)
      PRINT #1, I; TAB(10); USING PF1$; MCNP(I); TAB(20); SUMP; TAB(30);
         SUMP1; TAB(40); MCNO(I); TAB(50); SUMO; TAB(60); SUMO1
    NEXT I
  '-------
      SUM1 = MC1 + MC2P * 2 + MC2O * 2
      SUM = SUMP + SUMO + MC1 + MC2P + MC2O
      MC2T = MC2P + MC2O
      IF SUM - .001 >= 1 THEN GOTO 333
    NEXT CT1
333   PRINT #1, "-------------------------------------------------------------"
      PRINT #1, "Sum mi Selectivity  ="; SUM; CT1
      PRINT #1, "Sum mi Selectivity * No of carbon ="; SUMT + SUM1
      PRINT #1, "-------------------------------------------------------------"
       END SUB


SUB EngBL
'
  '-----------
    PRINT #1, "-------------------------------------------------------------"

    'Energy Balance Calculation ;ENG,(j/m^3.s)
    '----------------------------------------
    ENG1 = ES * EL * RP * DHR * RFT
    ENG2 = US / L * ((RSL * CpS * TRI) - (RSL * CpS * TR))
    ENG3 = HE * (TR - TC)
    'Calculation of Specific Cooling Area ;ACC,(1/m)
    '----------------------------------------------
    ACC = (ENG1 + ENG2) / ENG3
    PRINT #1, "Specific Cooling Area ;ACC,(1/m)="; ACC
 END SUB
```

```
    '-------------------------------------------------
    ACC = (ENG1 + ENG2) / ENG3
    PRINT #1, "Specific Cooling Area ;ACC,(1/m)="; ACC
    PRINT #1, "*************************************************************"

END SUB

SUB HeatCof
'-----------

    '"Calculation of Heat Transfer Coef ,HE ;(w.m^2/K)"
    '-------------------------------------------------------------

    HE1 = .1 * RSL * CpS * UG1
    HE2 = UG1 ^ 3 * RSL / (G * VS)
    HE3 = (VS * CpS / TCS) ^ 2
    HE = HE1 * ((HE2 * HE3) ^ -.25)
    PRINT #1,
    PRINT #1, "Heat Transfer Coef.;HE(w.m^2/K)="; HE
    PRINT #1, "-------------------------------------------------------------------"

END SUB

SUB HydPra
'-----------

    '"Calculation of Gas Hold up (Small &Large Bubble)""
    '---------------------------------------------------

    VD = UO * (1 + .8 * ES / UO)
    EDF = EDO * (RG / RGO) ^ .48 * (1 - .7 * ES / EDO)
    UDF = EDF * VD          'Superficial Velocity of Small Bubbles,(m/s)
    ULB = UG - UDF          'Superficial Velocity of Large Bubbles,(m/s")
    ELB = .3 * (ULB ^ .58) * ((RG / RGO) ^ .5)
    EG = ELB + EDF * (1 - ELB)                ' total gas hold up
    EL = 1 - ES - EG                          ' liquid hold up
    PRINT #1, "Superficial Velosity of Small Bubbles,UDF,(m/s)="; UDF
    PRINT #1, "Superficial Velosity of Large Bubbles,ULB,(m/s) = "; ULB
    PRINT #1, "Small Gas Hold up  ;EDF="; EDF
    PRINT #1, "Large Gas Hold up  ;ELB="; ELB
    PRINT #1, "Solid Hold up      ;ES="; ES
    PRINT #1, "Liquid Hold up     ;EL="; EL
    PRINT #1, "Total Gas Hold up  ;EG="; EG
    PRINT #1, "-------------------------------------------------"
    ' Calculation of Volumetric Mass Transfer Coef.,1/s""
    '----------------------------------------------------

FOR I = 1 TO NC
'--------------

    KLaS(I) = EDF * (DL(I) / DLO) ^ .5
    KLaL(I) = .5 * ELB * ((DL(I) / DLO) ^ .5)
    PRINT #1, "_____________________________________________________"
    PRINT #1, "Vol. Mass Trans Coef.for S Bubble(1/S):KLaS("; C$(I); ")=";
    KLaS(I)
    PRINT #1, "Vol. Mass Trans Co.for L Bubble(1/S):KLaL("; C$(I); ")="; KLaL(I)
NEXT I
'-------
END SUB
```

```
SUB InputData
'----------------

    PRINT "DATE  "; DATE$, "TIME  "; TIME$
    PRINT "======================"
    PRINT : INPUT "enter the data D_title;D_title$:", DTitle$
    PRINT "  REACTOR CONDITION"
    PRINT "-------------------------------------------"
    PRINT TR$; : INPUT TR
    PRINT TRI$; : INPUT TRI
    PRINT TC$; : INPUT TC
    PRINT P$; : INPUT P
    PRINT L$; : INPUT L
    PRINT D1$; : INPUT D1
    PRINT DHR$; : INPUT DHR
    PRINT RG$; : INPUT RG
    PRINT RGO$; : INPUT RGO
    PRINT ES$; : INPUT ES
    PRINT CF$; : INPUT CF
    PRINT UO$; : INPUT UO
    PRINT UG$; : INPUT UG
    PRINT US$; : INPUT US
    PRINT "LIQUID PROPERTIES"
    PRINT "_____________________
    PRINT RL$; : INPUT RL
    PRINT VL$; : INPUT VL
    PRINT TCL$; : INPUT TCL
    PRINT EDO$; : INPUT EDO
    PRINT CpL$; : INPUT CpL
    PRINT DLO$; : INPUT DLO
    PRINT "CATALYST PROPERTIER"
    PRINT "_____________________
    PRINT TCC$; : INPUT TCC
    PRINT CpC$; : INPUT CpC
    PRINT RP$; : INPUT RP
    PRINT RSK$; : INPUT RSK
    PRINT "FEED PROPERTIES"
    PRINT "-----------------"
    PRINT NC$; : INPUT NC
 FOR I = 1 TO NC

_________________
   PRINT "Input the Name of the Components in the Feed:C$("; I; ")=";
   INPUT C$(I)
   PRINT "Input the M.WT. of "; C$(I); "  in the Feed M.WT("; C$(I); ")=";
   INPUT MWT(I)
   PRINT "Input the Mole fr. of "; C$(I); "  in the Feed YO("; C$(I); ")=";
   INPUT YO(I)
   PRINT "Input Henery Coff. of "; C$(I); ",pa.m3/mol: HC("; C$(I); ") = ";
   INPUT HC(I)
   PRINT "Input the Diffusivity. of "; C$(I); ",(m/s^2),:DL("; C$(I); ")=";
   INPUT DL(I)
   PRINT " Input the Feed Ratio of the Component :F("; C$(I); ") = ";
   INPUT F(I)
 NEXT I
'
 ____________

  INPUT "Enter -1 if you want to save the data &0 if not ;dts:", DTS
  IF DTS THEN CALL SaveData
```

```
END SUB

SUB PhyProp
'
 ----------------


    'Calculation of Slurry Density,rsl,  kg/m^3"
   '-------------------------------------------------
    RSL = RL * (1 - RL * ES / RSK) + (RP * ES)
    PRINT #1, "Slurry Dinsity: RSL(kg/m^3)="; RSL
    PRINT #1,

   '"Calculation of Slurry Viscosity,:VS,(pa.s)"
   '-------------------------------------
     VS = VL * (1 + 4.5 * ES)
     PRINT #1, "Slurry Viscosity:vs(pa.s)="; VS
     PRINT #1,
   '"Calculation of Slurry Heat Capacity ,CpS ;(J/m3R)"
   '-----------------------------------------------------
     CpS = ES * RP / RL * CpC + (1 - (ES * RP / RL)) * CpL
     PRINT #1, "Slurry Heat Capacity:CpS(j/m3R)="; CpS

  '"Thermal Conductivity of Slurry  ;TCS ,(w/m.K)
   '-------------------------------------------------

    TCS1 = TCC + 2 * TCL - 2 * ES * (TCL - TCC)
    TCS2 = 2 * TCL + TCC + ES * (TCL - TCC)
    TCS = TCL * TCS1 / TCS2                  '"Thermal Conductivity of slurr
    PRINT #1, "Thermal Conductivity of Slurry;TCS(w/m.K)="; TCS
END SUB

SUB PrintData
  CLS : PRINT "the data title:"; titles
   PRINT "  REACTOR CONDITION"
   PRINT "DATE  "; DATE$, "TIME  "; TIME$
   PRINT "INPUT DATA PRINT OUT"
   PRINT "REACTOR CONDITIONS"
   PRINT "Reactor Temperature  ;TR,(K)="; TR
   PRINT "Reactor Inlet Temperature  ;TRI,(K):", TRI
   PRINT " Reaction Enthalpy  ;DHR,(J/mol)="; DHR
   PRINT "Reactor Length  ;L,(m)="; L
   PRINT "Reactor Length  ;D1,(m)="; D1
   PRINT "Reactor Pressure  ;P,(pa)="; P
   PRINT "Inlet Superfacial Velocity  ;UG,(m/s)="; UG
   PRINT "Density of Gas at Reactor Condition  ;RG,(kg/m^3)="; RG
   PRINT "Density of Gas at Ambient Condition ;RGO,(kg/m^3)="; RGO
   PRINT "Slurry Hold up  ;ES,(m^3l/m^3r)=:"; ES
   PRINT "Rise Vel. of the Small Bubbles at 0 Solids  ;UO,(m/s)=:"; UO
   PRINT "Cooling Temperature  ;TC,(K)=:"; TC
   PRINT "Contraction Factor ;CF=:"; CF
   PRINT "Slurry Velocity  ;US,(m/s)=:"; US
   PRINT "Diffusivity at Reference Condition  ;DLO,(m^2/s)=:"; DLO
   PRINT "Gravity  ;G,(m/s^2)=:"; G
   PRINT "LIQUID PROPERTIES"
   PRINT "Liquid Density  ;RL,(kg/m^3)="; RL
   PRINT "Refrence Hold up at Pure Liquid  ;EDO=:"; EDO
   PRINT "Liquid Viscosity  ;VL,(m/s)="; VL
   PRINT "Thermal Conductivity of Liquid   ;TCL,()="; TCL
```

```
   PRINT "Heat Capacity of Liquid    ;CpL,(j/kg.k))="; CpL
   PRINT "CATALYST PROPERTIES"
   PRINT "Catalyst Particle Density  ;RP,(kg/m^3) ="; RP
   PRINT "Skelton Density   ;RSK,(kg/m^3)="; RSK
   PRINT "Thermal Conductivity of Catalyst  ; TCC,(w/m.K):="; TCC
   PRINT "Heat Capacity of Catalyst   ;CpC,( j/(kg.k)):="; CpC
   PRINT " FEED PROPERTIES "
   PRINT "Gas Constant  ;R,(pa*m^3/(mol*K))="; R
   PRINT "No of Component  ;NC=:"; NC
 FOR I = 1 TO NC
'---------------
   PRINT "C$("; I; ")="; C$(I)
   PRINT "The Mol.WT.of "; C$(I); " in the Feed M.WT("; C$(I); ") = "; MWT(I)
   PRINT "The Mol.Fr.of "; C$(I); " in the Feed YO("; C$(I); ") = "; YO(I)
   PRINT "The Diffusivity for "; C$(I); ", dl("; C$(I); "),(m^2/s)="; DL(I)
   PRINT "Henery Co. for "; C$(I); ", HC("; C$(I); "),(Pa.m^3/mol)="; HC(I)
NEXT I
'--------
END SUB

SUB READDATA
'---------------
INPUT "Enter the drive name (drive:\)&file name to read the data:", DFileName$
OPEN DFileName$ FOR INPUT AS #4
   INPUT #4, DT$, TM$
   INPUT #4, DTitle$
   INPUT #4, TR, TRI, TC, P, L, D1, DHR, RG, RGO
   INPUT #4, ES, CF, UO, UG, US
   INPUT #4, RL, VL, TCL, EDO, CpL, DLO
   INPUT #4, TCC, CpC, RP, RSK, NC
 FOR I = 1 TO NC
'
 ----------------
   INPUT #4, C$(I)
   INPUT #4, MWT(I)
   INPUT #4, YO(I)
   INPUT #4, HC(I)
   INPUT #4, DL(I)
   INPUT #4, F(I)
 NEXT I
'
 ------------
 CLOSE #4
 END SUB

SUB Results
'
 ----------


 INPUT "Enter The Drive Name (Drive :\) &File name to Save Results(<=8chs.<=3"
 RFilename$
 INPUT "Enter the results titles:", RTITLE$
 OPEN RFilename$ FOR OUTPUT AS #5
   WRITE #5, "DATE  ", DATE$, "TIME  ", TIME$
   WRITE #5, "======================"
   WRITE #5, "The Data Used for Calculations"
   WRITE #5,
   WRITE #5, TR$, TR
   WRITE #5, TRI$, TRI
   WRITE #5, TC$, TC
   WRITE #5, P$, P
```

```
   WRITE #5, CpL$, CpL
   WRITE #5, DLO$, DLO
   WRITE #5, TCC$, TCC
   WRITE #5, CpC$, CpC
   WRITE #5, RP$, RP
   WRITE #5, RSK$, RSK
   WRITE #5, NC$, NC
 FOR I = 1 TO NC
'
 ------------------
   WRITE #5, "The Name of Component in the Feed ;C$(I) ", C$(I)
   WRITE #5, "The Mole Wieght ;M.WT(", C$(I), " )", MWT(I)
   WRITE #5, "The Mole Fraction in the Feed  ;YO(", C$(I), " )", YO(I)
   WRITE #5, "The Henery Coef. ,(pa.m3/mol) ;HC(", C$(I), ")", HC(I)
   WRITE #5, "The Diffusivity Coef of the Comp.;(m2/s) ;DL(", C$(I), ")", DL(I)
   WRITE #5, "The Diffusivity Coef of the Comp. ;(m2/s) ;F(", C$(I), ")", F(I)
 NEXT I
'
 ------------
 CLOSE #5
END SUB

  SUB RNX

    ' "Calculation of Kinetic Rate  ;RFT ,(mol/kg/s)
    PH2 = .4 * P * 10 ^ -5                          ' partial pressure of H2,(pa)
    PCO = .6 * P * 10 ^ -5                          '   "       "    " CO, (pa)
    PH2O = .00006 * P * 10 ^ -5                    ' partial pressure of H2O,(pa)
    PCO2 = .05 * P * 10 ^ -5                        '   "       "    " CO2, (pa)
    K1 = .0339: A = 1.185: B = .656: KW = .0292: K3 = 3.07: KP = 86
    PR1 = (1 + A * PCO + B * PCO2)
    RFT = K1 * (PH2 ^ .5) * PCO / (PR1 ^ 2)         ' kinetic rate,( mol/kg/s)
    PR2 = (PCO2 * PH2) / KP
    PR3 = (PCO + K3 * PH2O)
    RWGS = KW * (PCO * PH2O - PR2) / (PR3 ^ 2)       ' kinetic rate,( mol/kg/s)
    AL = .69: JM = .25
    MN = (1 - AL) ^ 2 + (JM * AL * (1 - AL))
    VHC1 = (1 - AL) / (3 + MN)
    VHC2 = (1 - AL) / (3 + MN)
    RX = (RFT + RWGS) * ES * EL * RP
    PRINT #1, "Kinetic Rate;RFT,(mol/kg/s)="; RFT
    PRINT #1, "Kinetic Rate;RWGS,(mol/kg/s)="; RWGS
    PRINT #1, "Kinetic Rate;RX="; RX
    PRINT #1, "Kinetic VHC1="; VHC1

END SUB

SUB SaveData
'----------------
INPUT "enter the drive (drive:\)&file name to save the data<=8chs.<=3):",
DFileName$
  OPEN DFileName$ FOR OUTPUT AS #3
  WRITE #3, DT$, TM$
  WRITE #3, DTitle$
  WRITE #3, TR, TRI, TC, P, L, D1, DHR, RG, RGO
  WRITE #3, ES, CF, UO, UG, US
  WRITE #3, RL, VL, TCL, EDO, CpL, DLO
  WRITE #3, TCC, CpC, RP, RSK, NC
FOR I = 1 TO NC
'
 ----------------
   WRITE #3, C$(I)
   WRITE #3, MWT(I)
   WRITE #3, YO(I)
```

```
    PRINT #1, "Kinetic Rate;RWGS,(mol/kg/s)="; RWGS
    PRINT #1, "Kinetic Rate;RX="; RX
    PRINT #1, "Kinetic VHC1="; VHC1

END SUB

SUB SaveData
'-----------------

CLS
INPUT "enter the drive (drive:\)&file name to save the data<=8chs.<=3):",
DFileName$

  OPEN DFileName$ FOR OUTPUT AS #3
  WRITE #3, DT$, TM$
  WRITE #3, DTitle$
  WRITE #3, TR, TRI, TC, P, L, D1, DHR, RG, RGO
  WRITE #3, ES, CF, UO, UG, US
  WRITE #3, RL, VL, TCL, EDO, CpL, DLO
  WRITE #3, TCC, CpC, RP, RSK, NC
FOR I = 1 TO NC
'  ----------------
   WRITE #3, C$(I)
   WRITE #3, MWT(I)
   WRITE #3, YO(I)
   WRITE #3, HC(I)
   WRITE #3, DL(I)
   WRITE #3, F(I)
 NEXT I
'  ------------

 CLOSE #3
END SUB

SUB TIME
     REM time subrotine
     REM --------------
     TT1 = VAL(LEFT$(TT1$, 2))
     TT2 = VAL(MID$(TT1$, 4, 2))
     TT3 = VAL(RIGHT$(TT1$, 2))
     TT4 = VAL(LEFT$(TT2$, 2))
     TT5 = VAL(MID$(TT2$, 4, 2))
     TT6 = VAL(RIGHT$(TT2$, 2))
     TT7 = TT6 + 60 * TT5 + 60 * 60 * TT4 - (TT3 + 60 * TT2 + 60 * 60 * TT1)
END SUB
```

RUN NO.: AF-R15.1C **TITLE: LIQUID PHASE FISCHER-TROPSCH (III) SYNTHESIS IN LAPORTE AFDU**

Start Date / Time	10/17/1996	12.00
End Date / Time	10/18/1996	12.00

On-stream Time From Start-up (hr)	
Start	64.00
End	88.00

Reaction Conditions:					
Temperature	average	deg F	440.1	deg C	226.7
Pressure	PIC-201	psig	710.0	bara	49.97
Space Velocity		sL/kg-hr	7612		
Superficial Gas Vel. - Inlet		ft/sec	0.43	cm/sec	13.18
(based on average reactor temp)					
Recycle Ratio			3.20		

Slurry Data:				
Catalyst Oxide Wt (Reactor)	lbs	860	kg	390.1
Slurry Concentration by NDG	wt%	42.4		
Slurry Concentration by DP	wt%	39.9		
Slurry Level by NDG % NDG Span		95.2		
Slurry Height	ft	20.57	meters	6.27
Average Gas Holdup by NDG	Vol%	41.4		
Average Gas Holdup by DP	Vol%	35.8		

Performance Results	
CO Conversion per pass, mole %	9.1
H2 Conversion per pass, mole %	15.8
CO + H2 Conversion per pass, mole %	13.0
Plant CO Conversion, mole%	36.8
Plant H2 Conversion, moie%	54.7
Plant CO+H2 Conversion, mole%	48.4
CO Conversion Rate, gmole CO converted/kg cat oxide-hr	11.6
HC Production Rate, grams of HC (CH2.1) produced/kg cat oxide-hr	163.4
Reactor Productivity (STY) grams of H C (CH2.1)/lit of reactor vol. - hr	43.85
H2/CO in Fresh Feed, mole/mole	1.82
H2/CO in Reactor Feed, mole/mole	1.41
H2/CO Usage Ratio, mole/mole	2.43
H2/CO in Outlet, mole/mole	1.30
CO2 Selectivity, mole %	0.41
HC Selectivity (CO2 free) wt%:	
CH4	13.88
C2H6	1.50
C2H4	1.01
C3H8	1.90
C3H6	3.57
SUM C4H10	2.57
SUM C4H8	3.40
SUM C5H11	5.47

Reactor Heat Balance	Btu/hr	kW
Chemical Heat Production by Reaction	708882	207.75
Sensible Gas Heat	-114281	-33.49
Sensible Oil Heat	-453176	-132.81
Sensible Wax Heat	-80173	-23.50
Estimate of Heat Loss from Catalyst Drying Data	-35000	-10.26
% Heat Balance based on Reaction Heat	96.30	

Mass Balance	Reactor lb/hr	Plant lb/hr	Feed lb/hr	Prod Gas lb/hr
Fresh Feed		823	823	
HP H2 Feed				
Recycle Feed			3317	3317
Reactor Feed	4162		4162	
Total In	4162	823		
Prod Gas	3839			3839
Main Purge		541		541
22.11 Purge	45.7	45.7		
HC Phase	36.9	36.9		
AQ Phase	200.1	200.1		
Heavy Wax	34.0	34.0		
Light Wax				
Total Out	4156	857		
Mass Balance, %	99.8	104.2	100.5	100.5

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RUN NO.: AF-R15.1C

TITLE: LIQUID PHASE FISCHER-TROPSCH (III) SYNTHESIS IN LAPORTE AFDU

Compositions (mole%):		LP FRESH FEED	HP FRESH FEED (H2)	RECYCLE FEED	REACTOR FEED GAS	PRODUCT GAS	MAIN (22.10) PURGE	22.11 PURGE	REACTOR OUTLET (estimated)
Components									
1	H2	62.08	100.00	50.14	52.89	50.14	50.14	48.34	48.04
2	N2	3.71	0.00	7.12	6.32	7.12	7.12	6.93	6.82
3	CO	34.20	0.00	38.47	37.62	38.47	38.47	38.24	36.85
4	CH4	0.00	0.00	2.93	2.18	2.93	2.93	3.12	2.81
5	CO2	0.00	0.00	0.12	0.09	0.12	0.12	0.16	0.11
6	ETHANE	0.00	0.00	0.17	0.13	0.17	0.17	0.23	0.16
7	ETHYLENE	0.00	0.00	0.02	0.00	0.02	0.02	0.03	0.02
8	PROPANE	0.00	0.00	0.15	0.11	0.15	0.15	0.29	0.14
9	PROPYLENE	0.00	0.00	0.27	0.20	0.27	0.27	0.51	0.26
10	ISOBUATNE	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
11	N-BUTANE	0.00	0.00	0.13	0.10	0.13	0.13	0.38	0.13
12	T-BUTENE-2	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
13	BUTENE-1	0.00	0.00	0.15	0.12	0.15	0.15	0.20	0.15
14	ISOBUTYLENE	0.00	0.00	0.00	0.00	0.00	0.00	0.24	0.00
15	C-BUTENE-2	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00
16	SUM C5	0.00	0.00	0.19	0.13	0.19	0.19	0.63	0.18
17	SUM C6	0.00	0.00	0.08	0.08	0.08	0.08	0.51	0.08
18	SUM C7	0.00	0.00	0.04	0.03	0.04	0.04	0.14	0.04
19	SUM C8	0.00	0.00	0.01	0.01	0.01	0.01	0.01	0.01
20	SUM C9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	SUM C10	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
	H2O								4.11
	HC								0.10
	LIGHT WAX								0.000
	TOTAL	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
Mole Wt	lb/lb mole	11.87	2.02	14.96	14.26	14.96	14.96	16.15	15.21
Flows	SCFH	26798.58	0.00	85721.03	112858.42	99218.39	13971.76	1093.39	103576.37
	lb mole/hr	69.31	0.00	221.70	291.89	256.61	36.14	2.83	267.88
	lb/hr	823.03	0.00	3316.81	4162.20	3839.06	540.61	45.68	4074.36
	Nm3/hr	705.24	0.00	2255.85	2970.01	2611.05	367.68	28.77	2725.74
	kgmol/hr	31.44	0.00	100.56	132.40	116.40	16.39	1.28	121.51
	kg/hr	373.32	0.00	1504.49	1887.96	1741.39	245.22	20.72	1848.12
Temperature	deg F	277.9	86.7	124.9	247.0	85.0	83.2	79.3	
	deg C	136.6	30.4	51.6	119.5	29.4	28.5	26.3	
Pressure	psig	762.5	780.5	818.1	749.6	662.2	671.6	26.9	
	bara	53.59	54.83	57.42	52.69	46.67	47.32	2.86	

RUN NO.: AF-R16.1B TITLE: LIQUID PHASE FISCHER-TROPSCH (IV) SYNTHESIS IN LAPORTE AFDU

Start Date / Time	04/03/1998	12.00
End Date / Time	04/04/1998	8.00

On-stream Time From Start-up (hr)	
Start	142.00
End	162.00

Reaction Conditions:					
Temperature	average	deg F	498.1	deg C	259.0
Pressure	PIC-201	psig	710.0	bara	49.97
Space Velocity		sL/kg-hr	14925		
Superficial Gas Vel. - Inlet (based on average reactor temp)		ft/sec	0.41	cm/sec	12.48
Recycle Ratio			1.14		

Slurry Data:				
Catalyst Oxide Wt (Reactor)	lbs	390	kg	176.9
Slurry Concentration by NDG	wt%	28.8		
Slurry Concentration by DP	wt%	27.7		
Slurry Level by NDG % NDG Span		96.5		
Slurry Height	ft	20.77	meters	6.33
Average Gas Holdup by NDG	Vol%	50.5		
Average Gas Holdup by DP	Vol%	47.3		

Performance Results	
CO Conversion per pass, mole %	33.1
H2 Conversion per pass, mole %	59.9
CO + H2 Conversion per pass, mole %	47.6
Plant CO Conversion, mole%	76.8
Plant H2 Conversion, mole%	91.3
Plant CO+H2 Conversion, mole%	86.3
CO Conversion Rate, gmole CO converted/kg cat oxide-hr	83.0
HC Production Rate, grams of HC (CH2.1) produced/kg cat oxide-hr	1155.1
Reactor Productivity (STY) grams of H C (CH2.1)/lit of reactor vol. - hr	139.23
H2/CO in Fresh Feed, mole/mole	1.88
H2/CO in Reactor Feed, mole/mole	1.17
H2/CO Usage Ratio, mole/mole	2.13
H2/CO in Outlet, mole/mole	0.70
CO2 Selectivity, mole %	1.33
HC Selectivity (CO2 free) wt%:	
CH4	13.95
C2H6	2.05
C2H4	0.08
C3H8	2.40
C3H6	1.46
SUM C4H10	1.89
SUM C4H8	1.24

Reactor Heat Balance	Btu/hr	kW
Chemical Heat Production by Reaction	2277851	667.57
Sensible Gas Heat	-118507	-34.73
Sensible Oil Heat	-1781173	-522.01
Sensible Wax Heat	-244482	-71.65
Estimate of Heat Loss from Catalyst Drying Data	-50000	-14.65
% Heat Balance based on Reaction Heat	96.33	

Mass Balance	Reactor lb/hr	Plant lb/hr	Feed lb/hr	Prod Gas lb/hr
Fresh Feed		1300	1300	
HP H2 Feed		89	89	
Recycle Feed			2790	2790
Reactor Feed	4202		4202	
Total In	4202	1390		
Prod Gas	3266			3266
Main Purge		481		481
22.11 Purge	0.0	0.0		
HC Phase	287.8	287.8		
AQ Phase	554.0	554.0		
Heavy Wax	59.2	59.2		
Light Wax				
Total Out	4167	1382		
Mass Balance, %	99.2	99.5	100.5	100.2

RUN NO.: AF-R16.1B

TITLE: LIQUID PHASE FISCHER-TROPSCH (IV) SYNTHESIS IN LAPORTE AFDU

Compositions (mole%):		LP FRESH FEED	HP FRESH FEED (H2)	RECYCLE FEED	REACTOR FEED GAS	PRODUCT GAS	MAIN (22.10) PURGE	22.11 PURGE	REACTOR OUTLET (estimated)
Components									
1	H2	43.59	100.00	28.14	44.25	28.14	28.14	8.18	23.35
2	N2	3.04	0.00	9.83	6.20	9.83	9.83	4.82	8.15
3	CO	53.37	0.00	40.06	37.72	40.06	40.G6	24.11	33.24
4	CH4	0.00	0.00	15.62	8.33	15.62	15.62	23.27	12.96
5	CO2	0.00	0.00	1.83	0.99	1.83	1.83	7.57	1.52
6	ETHANE	0.00	0.00	1.39	0.76	1.39	1.39	7.11	1.16
7	ETHYLENE	0.00	0.00	0.02	0.01	0.02	0.02	0.10	0.02
8	PROPANE	0.00	0.00	1.02	0.55	1.02	1.02	7.96	0.84
9	PROPYLENE	0.00	0.00	0.67	0.36	0.67	0.67	5.27	0.56
10	ISOBUATNE	0.00	0.00	0.01	0.00	0.01	0.01	0.09	0.01
11	N-BUTANE	0.00	0.00	0.46	0.24	0.46	0.46	4.03	0.38
12	T-BUTENE-2	0.00	0.00	0.04	0.02	0.04	0.04	0.31	0.03
13	BUTENE-1	0.00	0.00	0.26	0.12	0.26	0.26	2.33	0.22
14	ISOBUTYLENE	0.00	0.00	0.03	0.04	0.03	0.03	0.26	0.02
15	C-BUTENE-2	0.00	0.00	0.05	0.02	0.05	0.05	0.40	0.04
16	SUM C5	0.00	0.00	0.32	0.18	0.32	0.32	2.69	0.27
17	SUM C6	0.00	0.00	0.11	0.06	0.11	0.11	0.85	0.09
18	SUM C7	0.00	0.00	0.11	0.12	0.11	0.11	0.62	0.09
19	SUM C8	0.00	0.00	0.04	0.04	0.04	0.04	0.01	0.03
20	SUM C9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	SUM C10	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
	H2O								15.98
	HC								1.04
	LIGHT WAX								0.000
	TOTAL	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
Mole Wt	lb/lb mole	16.68	2.02	19.97	16.19	19.97	19.97	30.75	20.92
Flows	SCFH	30138.70	17101.00	54031.22	100355.33	63249.80	9314.22	0.00	76219.29
	lb mole/hr	77.95	44.23	139.74	259.55	163.59	24.09	0.00	197.13
	lb/hr	1300.26	89.34	2790.32	4201.68	3266.39	481.01	0.00	4123.30
	Nm3/hr	793.14	450.03	1421.90	2640.97	1664.49	245.11	0.00	2005.80
	kgmol/hr	35.36	20.06	63.39	117.73	74.20	10.93	0.00	89.42
	kg/hr	589.79	40.53	1265.68	1905.87	1481.62	218.19	0.00	1870.32
Temperature	deg F	266.7	82.5	98.2	238.1	75.5	74.4	73.4	
	deg C	130.4	28.0	36.8	114.5	24.2	23.5	23.0	
Pressure	psig	768.1	779.2	760.3	734.4	686.4	682.3	33.5	
	bara	53.97	54.74	53.43	51.65	48.34	48.06	3.32	

RUN NO.: AF-R16.1C TITLE: LIQUID PHASE FISCHER-TROPSCH (IV) SYNTHESIS IN LAPORTE AFDU

Start Date / Time	04/04/1998	8.00
End Date / Time	04/05/1998	4.00

On-stream Time From Start-up (hr)	
Start	162.00
End	182.00

Reaction Conditions:					
Temperature	average	deg F	498.0	deg C	258.9
Pressure	PIC-201	psig	710.0	bara	49.97
Space Velocity		sL/kg-hr	14975		
Superficial Gas Vel. - Inlet (based on average reactor temp)		ft/sec	0.41	cm/sec	12.45
Recycle Ratio			1.11		

Slurry Data:				
Catalyst Oxide Wt (Reactor)	lbs	388	kg	176.0
Slurry Concentration by NDG	wt%	28.6		
Slurry Concentration by DP	wt%	27.6		
Slurry Level by NDG	% NDG Span	96.5		
Slurry Height	ft	20.77	meters	6.33
Average Gas Holdup by NDG	Vol%	50.1		
Average Gas Holdup by DP	Vol%	47.3		

Performance Results	
CO Conversion per pass, mole %	33.2
H2 Conversion per pass, mole %	60.5
CO + H2 Conversion per pass, mole %	48.4
Plant CO Conversion, mole%	75.7
Plant H2 Conversion, mole%	90.4
Plant CO+H2 Conversion, mole%	85.3
CO Conversion Rate, gmole CO converted/kg cat oxide-hr	81.5
HC Production Rate, grams of HC (CH2.1) produced/kg cat oxide-hr	1132.6
Reactor Productivity (STY) grams of H C (CH2.1)/lit of reactor vol. - hr	135.79
H2/CO in Fresh Feed, mole/mole	1.88
H2/CO in Reactor Feed, mole/mole	1.26
H2/CO Usage Ratio, mole/mole	2.30
H2/CO in Outlet, mole/mole	0.75
CO2 Selectivity, mole %	1.41
HC Selectivity (CO2 free) wt%:	
CH4	14.61
C2H6	2.42
C2H4	0.15
C3H8	2.51
C3H6	1.69
SUM C4H10	1.90
SUM C4H8	1.21

Reactor Heat Balance	Btu/hr	kW
Chemical Heat Production by Reaction		
Sensible Gas Heat		
Sensible Oil Heat		
Sensible Wax Heat		
Estimate of Heat Loss from Catalyst Drying Data		
% Heat Balance based on Reaction Heat		

Mass Balance	Reactor lb/hr	Plant lb/hr	Feed lb/hr	Prod Gas lb/hr
Fresh Feed		1301	1301	
HP H2 Feed		89	89	
Recycle Feed			2641	2641
Reactor Feed	4039		4039	
Total In	4039	1390		
Prod Gas	3138			3138
Main Purge		498		498
22.11 Purge	0.0	0.0		
HC Phase	275.8	275.8		
AQ Phase	531.0	531.0		
Heavy Wax	52.7	52.7		
Light Wax				
Total Out	3997	1357		
Mass Balance, %	99.0	97.6	100.2	100.0

RUN NO.: AF-R16.1C TITLE: LIQUID PHASE FISCHER-TROPSCH (IV) SYNTHESIS IN LAPORTE AFDU

Compositions (mole%):		LP FRESH FEED	HP FRESH FEED (H2)	RECYCLE FEED	REACTOR FEED GAS	PRODUCT GAS	MAIN (22.10) PURGE	22.11 PURGE	REACTOR OUTLET (estimated)
Components									
1	H2	43.54	100.00	29.59	46.37	29.59	29.59	9.41	24.58
2	N2	3.07	0.00	9.39	5.82	9.39	9.39	4.57	7.80
3	CO	53.39	0.00	39.71	36.78	39.71	39.71	25.39	32.99
4	CH4	0.00	0.00	15.15	7.81	15.15	15.15	21.44	12.59
5	CO2	0.00	0.00	1.73	0.90	1.73	1.73	6.67	1.44
6	ETHANE	0.00	0.00	1.38	0.71	1.38	1.38	7.24	1.15
7	ETHYLENE	0.00	0.00	0.02	0.00	0.02	0.02	0.11	0.02
8	PROPANE	0.00	0.00	1.01	0.53	1.01	1.01	8.18	0.84
9	PROPYLENE	0.00	0.00	0.67	0.34	0.67	0.67	5.28	0.55
10	ISOBUATNE	0.00	0.00	0.01	0.00	0.01	0.01	0.10	0.01
11	N-BUTANE	0.00	0.00	0.47	0.24	0.47	0.47	4.31	0.39
12	T-BUTENE-2	0.00	0.00	0.04	0.02	0.04	0.04	0.31	0.03
13	BUTENE-1	0.00	0.00	0.26	0.13	0.26	0.26	2.38	0.22
14	ISOBUTYLENE	0.00	0.00	0.03	0.02	0.03	0.03	0.28	0.03
15	C-BUTENE-2	0.00	0.00	0.05	0.02	0.05	0.05	0.41	0.04
16	sum C5	0.00	0.00	0.33	0.18	0.33	0.33	2.88	0.28
17	SUM C6	0.00	0.00	0.12	0.07	0.12	0.12	0.90	0.10
18	SUM C7	0.00	0.00	0.02	0.02	0.02	0.02	0.14	0.02
19	SUM C8	0.00	0.00	0.01	0.02	0.01	0.01	0.02	0.01
20	SUM C9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	SUM C10	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
	H2O								15.90
	HC								1.01
	LIGHT WAX								0.000
	TOTAL	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
Mole Wt	lb/lb mole	16.69	2.02	19.56	15.59	19.56	19.56	30.43	20.55
Flows	SCFH	30132.03	17104.10	52207.22	100178.56	62030.75	9842.83	0.00	74659.86
	lb mole/hr	77.93	44.24	135.03	259.10	160.43	25.46	0.00	193.10
	lb/hr	1301.01	89.36	2640.99	4039.26	3137.93	497.92	0.00	3968.45
	Nm3/hr	792.96	450.12	1373.90	2636.32	1632.41	259.03	0.00	1964.76
	kgmol/hr	35.35	20.07	61.25	117.53	72.77	11.55	0.00	87.59
	kg/hr	590.13	40.53	1197.94	1832.20	1423.36	225.85	0.00	1800.08
Temperature	deg F	272.0	85.2	104.2	238.7	83.8	81.3	69.3	
	deg C	133.4	29.6	40.1	114.8	28.8	27.4	20.7	
Pressure	psig	766.0	792.3	758.4	733.1	685.8	682.0	33.4	

RUN NO.: AF-R16.3A TITLE: LIQUID PHASE FISCHER-TROPSCH (IV) SYNTHESIS IN LAPORTE AFDU

Start Date / Time	0/06/1998	23.00
End Date / Time	04/07/1998	8.00

On-stream Time From Start-up (hr)	
Start	225.00
End	234.00

Reaction Conditions:					
Temperature	average	deg F	502.2	deg C	261.2
Pressure	PIC-201	psig	710.1	bara	49.98
Space Velocity		sL/kg-hr	22223		
Superficial Gas Vel. - Inlet (based on average reactor temp)		ft/sec	0.60	cm/sec	18.32
Recycle Ratio			2.12		

Slurry Data:				
Catalyst Oxide Wt (Reactor)	lbs	383	kg	173.7
Slurry Concentration by NDG	wt%	28.6		
Slurry Concentration by DP	wt%	27.3		
Slurry Level by NDG	% NDG Span	96.8		
Slurry Height	ft	20.81	meters	6.34
Average Gas Holdup by NDG	Vol%	50.2		
Average Gas Holdup by DP	Vol%	47.2		

Performance Results	
CO Conversion per pass, mole %	20.2
H2 Conversion per pass, mole %	43.0
CO + H2 Conversion per pass, mole %	32.2
Plant CO Conversion, mole%	70.2
Plant H2 Conversion, mole%	87.2
Plant CO+H2 Conversion, mole%	81.2
CO Conversion Rate, gmole CO converted/kg cat oxide-hr	76.9
HC Production Rate, grams of HC (CH2.1) produced/kg cat oxide-hr	1067.3
Reactor Productivity (STY) grams of H C (CH2.1)/lit of reactor vol. - hr	126.07
H2/CO in Fresh Feed, mole/mole	1.82
H2/CO in Reactor Feed, mole/mole	1.10
H2/CO Usage Ratio, mole/mole	2.34
H2/CO in Outlet, mole/mole	0.78
CO2 Selectivity, mole %	1.55
HC Selectivity (CO2 free) wt%:	
CH4	17.67
C2H6	2.48
C2H4	-0.05
C3H8	2.64
C3H6	1.73
SUM C4H10	1.55
SUM C4H8	1.45

Reactor Heat Balance	Btu/hr	kW
Chemical Heat Production by Reaction	2068071	606.09
Sensible Gas Heat	-178235	-52.24
Sensible Oil Heat	-1608608	-471.43
Sensible Wax Heat	-222668	-65.26
Estimate of Heat Loss from Catalyst Drying Data	-50000	-14.65
% Heat Balance based on Reaction Heat	99.59	

Mass Balance	Reactor lb/hr	Plant lb/hr	Feed lb/hr	Prod Gas lb/hr
Fresh Feed		1312	1312	
HP H2 Feed		86	86	
Recycle Feed			4882	4882
Reactor Feed	6296		6296	
Total In	6296	1398		
Prod Gas	5472			5472
Main Purge		590		590
22.11 Purge	0.0	0.0		
HC Phase	274.0	274.0		
AQ Phase	527.4	527.4		
Heavy Wax	8.6	8.6		
Light Wax				
Total Out	6282	1400		
Mass Balance, %	99.8	100.1	100.3	100.0

RUN NO.: AF-R16.3A TITLE: LIQUID PHASE FISCHER-TROPSCH (IV) SYNTHESIS IN LAPORTE AFDU

Compositions (mole%):		LP FRESH FEED	HP FRESH FEED (H2)	RECYCLE FEED	REACTOR FEED GAS	PRODUCT GAS	MAIN (22.10) PURGE	22.11 PURGE	REACTOR OUTLET (estimated)
Components									
1	H2	43.25	100.00	31.65	42.08	31.65	31.65	10.91	28.62
2	N2	3.06	0.00	7.73	5.86	7.73	7.73	4.08	6.99
3	CO	53.69	0.00	40.33	38.30	40.33	40.33	27.97	36.47
4	CH4	0.00	0.00	14.57	9.83	14.57	14.57	19.11	13.18
5	CO2	0.00	0.00	1.45	0.98	1.45	1.45	5.05	1.31
6	ETHANE	0.00	0.00	1.30	0.90	1.30	1.30	7.26	1.18
7	ETHYLENE	0.00	0.00	0.02	0.02	0.02	0.02	0.10	0.02
8	PROPANE	0.00	0.00	0.98	0.88	0.98	0.98	8.24	0.89
9	PROPYLENE	0.00	0.00	0.59	0.40	0.59	0.59	4.84	0.54
10	ISOBUTANE	0.00	0.00	0.01	0.01	0.01	0.01	0.10	0.01
11	N-BUTANE	0.00	0.00	0.48	0.33	0.48	0.48	4.53	0.44
12	T-BUTENE-2	0.00	0.00	0.05	0.03	0.05	0.05	0.42	0.04
13	BUTENE-1	0.00	0.00	0.24	0.16	0.24	0.24	2.20	0.22
14	ISOBUTYLENE	0.00	0.00	0.03	0.02	0.03	0.03	0.30	0.03
15	C-BUTENE-2	0.00	0.00	0.08	0.04	0.06	0.06	0.52	0.05
16	SUM C5	0.00	0.00	0.36	0.25	0.36	0.36	3.16	0.33
17	SUM C6	0.00	0.00	0.13	0.09	0.13	0.13	1.05	0.11
18	SUM C7	0.00	0.00	0.02	0.01	0.02	0.02	0.15	0.01
19	SUM C8	0.00	0.00	0.00	0.01	0.00	0.00	0.01	0.00
20	SUM C9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
21	SUM C10	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
	H2O								8.97
	HC								0.61
	LIGHT WAX								0.000
	TOTAL	100.00	100.00	100.00	100.00	100.00	100.00	100.00	100.00
Mole Wt	lb/lb mole	16.77	2.02	19.04	16.59	19.04	19.04	30.30	19.69
Flows	SCFH	30245.09	16504.40	99154.37	148743.26	111147.37	11978.68	0.00	122926.70
	lb mole/hr	78.22	42.69	256.45	379.53	287.47	30.98	0.00	317.93
	lb/hr	1311.76	86.23	4881.66	6296.36	5472.11	589.75	0.00	6261.44
	Nm3/hr	795.94	434.33	2609.37	3861.73	2924.98	315.23	0.00	3234.96
	kgmol/hr	35.48	19.36	116.32	172.15	130.39	14.05	0.00	144.21
	kg/hr	595.01	39.11	2214.31	2856.01	2482.13	267.51	0.00	2840.17
Temperature	deg F	279.1	80.1	122.8	295.2	85.2	82.7	73.2	
	deg C	137.3	26.7	50.4	146.2	29.6	28.2	22.9	
Pressure	psig	815.1	812.4	824.8	770.9	640.5	633.4	33.3	
	bara	57.21	57.02	57.88	54.17	45.17	44.68	3.31	

جامعة المنيا

كلية الهندسة

قسم الهندسة الكيميائية

ترشيد الطاقة والنمذجة لتحويل الغاز الطبيعى إلى وقود سائل باستخدام تكنولوجيا فيشر وتربش

دراسة مقدمة من

المهندس / حسين عبد الموجود محمد السيد

للحصول على درجة الدكتوراه

فى

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٢٠٠٥

الملخص العربى

هذه الدراسة نتناول طرق توفير الطاقة فى المراحل المختلفة لتحويل الغاز الطبيعى الى وقود سائل (GTL) والمعروفة بتكنولوجيا فيشر وتربش. وكذلك يتم تناول عملية النمذجة لنفس التكنولوجيا.

١-ففى مرحلة تحضير غاز التخليق تعتبر فكرة التخليق ذاتي الحرارة (Autothermal) وفيها يتم الجمع بين التخليق البخاري [Steam reforming] والأكسدة الجزئية (Partial Oxidation) خطوة هامة لتوفير الطاقة فى هذه المرحلة، حيث يتم الاستفادة من الحرارة الناتجة من عملية الأكسدة الجزئية (وهو تفاعل طارد للحرارة) لامداد الحرارة اللازمة لعملية التخليق البخاري (وهو تفاعل ماص للحرارة) ، وفى نفس الوقت يمكن إنتاج غاز التخليق بالنسبة المطلوبة (هيدروجين /أول أكسيد الكربون) اللازمة لعملية الفيشر و تربش.

عملية التكامل بين الثلاث خطوات اللازمة لعملية الفيشر وتربش يمكن ان ينتج عنها توفير فى الغاز الطبيعي ومن ثم الطاقة . كذلك فإن عملية الفيشر وتربش ذات الاتجاه الواحد بدون دوران للغازات التى لم تتفاعل يمكن ان ينتج عنها الطاقة البخارية اللازمة للعمليات الصناعية بالإضافة الى الطاقة الكهربائية حيث يمكن استخدام التوربينات الغازية الى جانب التوربينات البخارية فى عملية الدورة المشتركة (Combined Cycle) لتوليد الكهرباء والتى تحسن من اقتصاديات العملية.

وقد تم تناول عملية توفير الطاقة فى وحدة تجارب نصف صناعية لعملية الفيشر وتربش والتىاجريت فىوحدة تطوير انتاج الوقود البديل (AFDU) فى Laporte تكساس بأمريكا وذلك باستخدام برنامج تم تصميمه بمعهد بحوث البترول وهو برنامج (AMU) الذى يقوم بالاستعانة بدرجات الحرارة الخاصة بالمسارات الباردة والساخنة فى تقسيم النطاق الحراري الى مراحل مستقلة ثم يقوم البرنامج بكتابة معادلات التوازن الحراري لكل مرحلة بطريقة البرمجة الخطية وتحل هذه المعادلات بالبرنامج القياسي (LINDO) للحصول على اقل كميات من الطاقة المطلوبة سواء للتبريد او التسخين عند فرق معين من درجة حرارة التقارب (ΔT_{min}) .

وقد تم اخذ خمس فروق لدرجات حرارة تقارب ΔT_{min} وهى (١٠، ٢٠، ٣٠، ٤٠، ٥٠ $^{\circ}$م)

لتحديد فرق درجة الحرارة المثلى (optimum ΔT_{min}) الذى يصاحب اقل تكلفة كلية. وقد أوضحت النتائج ان الطاقة اللازمة للتسخين يمكن الاستغناء عنها كليه حتى فروق درجات حرارة٣٠ ° م ، حيث أتضح ان المحتوى الحراري للمسارات الساخنة كافياً لكى يعوض النقص فى المحتوى الحراري للمسارات الباردة ونحتاج فقط للطاقة اللازمة للتبريد وتم تصميم شبكة المبادلات الحرارية لكل حالة وحساب تكلفة المبدلات الحرارية عند نفس فروق درجات الحرارة . وأدت النتائج الى انه عند فرق درجات حرارة ١٠ ° م (ΔT_{min} =10 °c) يتم توفير أقصى طاقة وتحقيق اقل تكلفة.

٢-يمثل مفاعل المعلق ذو الفقاعات الانبوبى الاختيار الامثل لمعظم التكنولوجيات الحديثة بوجه عام فى عمليات تحويل الغازالطبيعى الى وقود سائل (فيشر وتربش) وكذلك فى اكبر شركتين فى هذا المجال وهما [ExxonMobil , Sasol] .

وتناولت الرسالة تصميم برنامج [نمذجة] لعملية الفيشر تربش حيث ان المفاعلات المعلقة ذات الفقاعات الأنبوبية معقدة ومتشابكة وتحتوى على اطوار المادة الثلاث التى تتمثل فى الطور الغازى [غاز التخليق] والطور السائل (السائل الناتج من التفاعل) والطور الصلب (العامل الحفاز).

وعمل نموذج لهذا المفاعل يتطلب معرفة كيناتيكية التفاعل (Kinetics) والحالة الحركية والهيدروديناميكية (Hydrodynamics) لهذه الأطوار الثلاثة داخل المفاعل ، ومعرفة توزيع المنتجات الناتجة من التفاعل (Product selectivity) .

وقد تم اختيار نموذج [Shah et al. , 1985] والذى تم تعديله بواسطة [Van der Laan , 1999] وهو يتميز بوجود نوعين من الفقاعات [الصغيرة والكبيرة] ، وتكون فيه الفقاعات الصغيرة مختلطة تماماً (Completely mixed) والفقاعات الكبيرة غير مختلطة (حالة سريان الدفعة- Plug flow) اما السائل الناتج وحبيبات العامل الحفاز فيكونا فى حالة مختلطة تماماً (Completely mixed).

تم حل معادلات النموذج بالطريقة التحليلية وبشكل عام فإن البرنامج الرئيسي الذي تم تصميمه (Software) ينادى البرامج الفرعية (Subroutines) اللازمة لحساب الحالة الهيدروديناميكية وكيناتيكا التفاعل وفى نفس الوقت يقوم بالحسابات الرئيسية لحل النموذج المطلوب .

نم استخدام البرنامج (Software) الذي تم تصميمه وتطويره في استرجاع نتائج البحث الذي قام به (Van der Laan , 1999) على مفاعل صناعي لمعرفة مدى صحة طريقة الحل التي تم استنباطها لحل المعادلات حيث استخدام الحديد كعامل حفاز . وذلك تحت تأثير عوامل تشغيلية مختلفة. وقد تم دراسة تأثير سرعة الغاز[Superficial gas velocity] وتركيز العامل الحفاز (Solid hold up) ونسبة الهيدروجين / أول أكسيد الكربون (Feed ratio) على نسبة تحويل الهيدروجين أول أكسيد الكربون ألي مواد هيدروكربونية وكمية المنتج من التفاعل (Hydrocarbons productivity) . ووجد أن تحويل غاز التخليق ألي مواد هيدروكربونية يتناقص بزيادة سرعة الغاز الداخل ألي المفاعل وتقليل نسبة هيدروجين/أول أكسيد الكربون ، وكذلك تقليل تركيز العامل الحفار أما كمية المنتج من التفاعل فتزيد بزيادة المتغيرات السابقة . وقد وجد آن النتائج متشابهة مع التي حصل عليها (Van der Laan , 1999) وكذلك تم حساب توزيع المنتجات (product selectivity) باستخدام نموذج (Van der Laan , 1999 (OPDRM)) وذلك مع تغيير نسبة (H_2/CO) في غاز التخليق وقد أعطى البرنامج نتائج مشابهة لتلك التي حصل عليه (Vander Laan, 1999) مما يعزز صحة البرنامج وطريقة الحل المقترحة.

٣-وقد استخدم نفس النموذج (البرنامج) ولكن باستخدام الكوبلت كعامل حفاز بدلاً من الحديد وذلك لتطبيقه على التجارب النصف صناعية بوحدة (AFDU) المشار اليها سلفاً. وفد قورنت نتائج البرنامج مع النتائج التجريبية تحت ظروف تشغيلية مختلفة وتم استخدام نموذج (OPDRM) بعد إجراء بعض التعديلات عليه وقد حصلنا من البرنامج على نتائج متوافقة مع تلك الموجودة والناتجة من التجارب المعملية من حيث كمية الغاز المحتجز ، وتوزيع المنتجات ونسبة تحويل كل من H_2 ، CO ، وكمية الناتج من التفاعل فى كل حالة.