Appendix A: ASPEN Plus Input File Gasifier Fortran Subroutine

Appendix A: ASPEN Plus Input File

```
DEF-STREAMS MIXCINC ALL

DIAGNOSTICS
   HISTORY SYS-LEVEL=4 SIM-LEVEL=4 PROP-LEVEL=2 STREAM-LEVEL=4
   MAX-PRINT SIM-LIMIT=5000 PROP-LIMIT=50

RUN-CONTROL MAX-ERRORS=500

DATABANKS PURECOMP / AQUEOUS / SOLIDS / INORGANIC / &
      ASPENPCD

PROP-SOURCES PURECOMP / AQUEOUS / SOLIDS / INORGANIC / &
      ASPENPCD .

;
;=============================================================================
;                          Components
;=============================================================================
;

COMPONENTS
   TAR C10H8 TAR /
   H2 H2 H2 /
   O2 O2 O2 /
   N2 N2 N2 /
   CO2 CO2 CO2 /
   CO CO CO /
   H2O H2O H2O /
   CH4 CH4 CH4 /
   H2S H2S H2S /
   NH3 H3N NH3 /
   COS COS COS /
   SO2 O2S SO2 /
   SO3 O3S SO3 /
   O2SI SIO2 O2SI /
   NO2 NO2 NO2 /
   NO NO NO /
   PHENOL C6H6O PHENOL /
   C6H6 C6H6 C6H6 /
   C2H6 C2H6 C2H6 /
   C2H4 C2H4 C2H4 /
   C2H2 C2H2 C2H2 /
   CARBON C CARBON /
   SULFUR S SULFUR /
   WOOD * WOOD /
   ASH * ASH /
   CHAR * CHAR
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;
;=============================================================================
;                          Flowsheet
;=============================================================================
;

FLOWSHEET MAIN
   BLOCK FEEDMIX IN=GASIFSTM WOOD SAND OUT=GFEED
   BLOCK GASIFIER IN=GFEED OUT=WOODGAS QGAS
   BLOCK CHARSEP IN=WOODGAS OUT=CHAR SYNGAS
   BLOCK CHARDEC IN=CHAR OUT=CHARCOMP QCHAR
   BLOCK AIRHEAT IN=COMBAIR2 OUT=HCOMBAIR QAIR
   BLOCK CHARFURN IN=CHARCOMP HCOMBAIR SANDSUPP QCHAR OUT= &
      COMBPROD QCOMB
   BLOCK COMBSPLT IN=COMBPROD OUT=CHARFLUE ASHSAND
   BLOCK SANDSPLT IN=ASHSAND OUT=SAND SANDPURG
   BLOCK SYNCOMPR IN=TOCOMPR OUT=SYNCOMPD 205
   BLOCK PRIMARY IN=TOREFHOT REFSTM OUT=SYNREFRM 105
   BLOCK HTSHIFT IN=TOHT OUT=FROMHT QHT
   BLOCK LTSHIFT IN=TOLT OUT=FROMLT QLT
   BLOCK REFHTR IN=207 OUT=TOREFHOT 198
   BLOCK WATPUMP IN=REFSTMA OUT=REFSTMB
   BLOCK WOODSEP IN=ARWOOD OUT=WOODWAT MIDWOOD
   BLOCK DRY2 IN=MIDWOOD WETDAIR OUT=DRYWOOD
   BLOCK DRY1 IN=WOODWAT FLUENAIR OUT=WETDAIR
   BLOCK DRYRMIX IN=CHARFLUE DRYRAIR2 OUT=FLUENAIR
   BLOCK PSA IN=TOPSAB OUT=H2PURIFY OFFGAS
   BLOCK OFFCOMB IN=OFFGAS OFFAIR2 105 OUT=OFFFLUE1
   BLOCK GSTMGEN IN=SYNREFRM GSTMIN OUT=FROMPRIM GASIFSTM
   BLOCK AIRCOMP1 IN=COMBAIR OUT=COMBAIR2
   BLOCK AIRCOMP2 IN=DRYRAIR OUT=DRYRAIR2
   BLOCK DRYRSEP IN=DRYWOOD OUT=DRIED GASWAT
   BLOCK MODEL1 IN=HOTIN COLDIN OUT=HOTOUT COLDOUT
   BLOCK SYNCOOL1 IN=SYNGAS OUT=SYNCOLD 197
   BLOCK MODEL2 IN=HI CI OUT=HO CO
   BLOCK LTCOOL IN=FROMHT 196 OUT=TOLT STEAM6
   BLOCK OFFCOMPR IN=OFFAIR1 OUT=OFFAIR2
   BLOCK REFSTM IN=REFSTMB OUT=REFSTM 135
   BLOCK COMBCOOL IN=OFFFLUE1 135 OUT=OFFFLUE2
   BLOCK HTCOOL IN=FROMPRIM OUT=TOHT
   BLOCK PUMP1 IN=BFW1A OUT=145
   BLOCK INTER2A IN=GAS2A 160 OUT=COOLED2A STEAM2A
   BLOCK INTER2B IN=GAS2B 165 OUT=COOLED2B STEAM2B
   BLOCK PUMP4 IN=BFW2A OUT=160
   BLOCK PUMP5 IN=BFW2B OUT=165
   BLOCK RECMIX IN=TOPSAA H2RECYCL OUT=TOPSAB
   BLOCK RECSPLT IN=H2PURIFY OUT=H2PROD H2RECYCL
   BLOCK STMGEN6 IN=OFFFLUE2 188 OUT=OFFFLUE3 STEAM4
   BLOCK B13 IN=BFW4 OUT=188
   BLOCK B3 IN=BFW6 OUT=196
   BLOCK B1 IN=SYNCOLD OUT=KOWATER TOCOMPR
   BLOCK B2 IN=SYNCOMPD 208 205 OUT=207
   BLOCK B5 IN=KOWATER OUT=208
   BLOCK PSACOOL IN=FROMLT 212 OUT=TOPSAA STEAM5 189
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    BLOCK B7 IN=BFW5 OUT=212
    BLOCK B4 IN=GAS1A OUT=COOLED1A 213
    BLOCK B6 IN=145 213 OUT=STMWAT
    BLOCK STMFLASH IN=STMWAT OUT=STEAM1A WAT1A

;
;=============================================================================
;                        Physical Property Data
;=============================================================================
;

PROPERTIES SYSOP3

PROP-REPLACE SYSOP3 RKS-BM
    PROP MUVMX MUVMX02
    PROP MULMX MULMX02
    PROP KVMX KVMX02
    PROP KLMX KLMX01
    PROP DV DV01
    PROP MUL MUL01
    PROP MUV MUV01
    PROP KV KV01
    PROP KL KL01

;

NC-COMPS WOOD ULTANAL SULFANAL PROXANAL

NC-PROPS WOOD ENTHALPY HCJ1BOIE / DENSITY DCOALIGT

NC-COMPS ASH GENANAL ULTANAL SULFANAL PROXANAL

NC-PROPS ASH ENTHALPY HCJ1BOIE / DENSITY DNSTYGEN

NC-COMPS CHAR ULTANAL SULFANAL PROXANAL

NC-PROPS CHAR ENTHALPY HCJ1BOIE / DENSITY DCHARIGT

PROP-DATA DATA1
    IN-UNITS ENG
    PROP-LIST DGSFRM / DHSFRM / MW
    PVAL O2SI .0 / .0 / 60.0860
    PVAL CARBON .0 / .0 / 12.0110
    PVAL SULFUR .0 / .0 / 32.0640

;
;=============================================================================
;                  Conventional Component Property Data
;=============================================================================
;

PROP-DATA DATA5
    IN-UNITS SI TEMPERATURE=F
    PROP-LIST VSPOLY
```

```
   PVAL CARBON .005340 .0 .0 .0 .0 .0 2500.0
   PVAL SULFUR .01550 .0 .0 .0 .0 .0 2500.0

PROP-DATA U-1
   IN-UNITS ENG MOLE-HEAT-CA='CAL/MOL-K' TEMPERATURE=K
   PROP-LIST CPSPO1
   PVAL CARBON 2.6730 .0026170 .0 .0 -116900.0 .0 273.0  &
      1373.0
   PVAL O2SI 12.80 .004470 .0 .0 -302000.0 .0 273.0 1973.0
   PVAL SULFUR 3.630 .00640 0.0 0.0 0.0 0.0 0.0 1000.000

PROP-DATA U-2
   IN-UNITS SI
   PROP-LIST DENGEN
   PVAL ASH 2000.0 .0 .0 .0

;
;=============================================================================
;                          Stream Structure
;=============================================================================
;

PROP-SET PS-1 CP RHO UNITS='BTU/LB-R' 'GM/CC' 'LB/CUFT'  &
      SUBSTREAM=MIXED COMPS=O2SI CARBON SULFUR PHASE=S

PROP-SET PS-2 DENSITY HEAT-CAP UNITS='LB/CUFT' 'GM/CC'  &
      'BTU/LB-R' 'CAL/GM-K' SUBSTREAM=NC COMPS=WOOD ASH CHAR  &
      PHASE=S

STREAM 207

STREAM ARWOOD
   SUBSTREAM MIXED TEMP=59 PRES=14.696
   MASS-FLOW H2O .78
   SUBSTREAM NC TEMP=59 PRES=14.696
   MASS-FLOW WOOD 1
   COMP-ATTR WOOD ULTANAL ( .920 50.880 6.04 .17 0 0.09  &
      41.9 )
   COMP-ATTR WOOD SULFANAL ( .450 .02250 .02250 )
   COMP-ATTR WOOD PROXANAL ( 11 15.29 83.52 .87 )

STREAM BFW1A
   SUBSTREAM MIXED TEMP=170 PRES=30
   MASS-FLOW H2O .8

STREAM BFW2A
   SUBSTREAM MIXED TEMP=59 PRES=30
   MASS-FLOW H2O .0565

STREAM BFW2B
   SUBSTREAM MIXED TEMP=59 PRES=30
   MASS-FLOW H2O .04825

STREAM BFW4
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   SUBSTREAM MIXED TEMP=59 PRES=30
   MASS-FLOW H2O .378

STREAM BFW5
   SUBSTREAM MIXED TEMP=59 PRES=30
   MASS-FLOW H2O .75

STREAM BFW6
   SUBSTREAM MIXED TEMP=59 PRES=14.696
   MASS-FLOW H2O .2

STREAM CI
   SUBSTREAM MIXED TEMP=59 PRES=30
   MASS-FLOW H2O .570

STREAM COLDIN
   SUBSTREAM MIXED TEMP=228 PRES=530
   MASS-FLOW TAR .014 / H2 .012 / CO2 .16 / CO .327 /  &
      H2O .51 / CH4 .069 / H2S .001 / NH3 .002 / C2H6  &
      .004 / C2H4 .035 / C2H2 .003

;

STREAM COMBAIR
   SUBSTREAM MIXED TEMP=59.0 PRES=14.696 MASS-FLOW=1.80
   MOLE-FRAC O2 .207340 / N2 .782180 / CO2 .000330 / H2O  &
      .010150

STREAM DRYRAIR
   SUBSTREAM MIXED TEMP=59 PRES=14.696 MASS-FLOW=6
   MOLE-FRAC O2 .207340 / N2 .782180 / CO2 .000330 / H2O  &
      .010150

STREAM GAS1A
   SUBSTREAM MIXED TEMP=397.8549 PRES=45.37759
   MASS-FLOW TAR .013804 / H2 .011585 / CO2 .160307 / CO  &
      0.327241 / H2O .50999 / CH4 .068728 / H2S .000781 /  &
      NH3 .001718 / C2H6 .003747 / C2H4 .035058 / C2H2  &
      .00254

STREAM GAS2A
   SUBSTREAM MIXED TEMP=414.9241 PRES=72.99842
   MASS-FLOW O2 .250564 / N2 .827514 / CO2 .000548 / H2O  &
      .006906

STREAM GAS2B
   SUBSTREAM MIXED TEMP=373.9805 PRES=162.6937
   MASS-FLOW O2 .250564 / N2 .827514 / CO2 .000548 / H2O  &
      .006906

;

STREAM GASIFSTM
   SUBSTREAM MIXED TEMP=1000 PRES=25
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   MASS-FLOW H2O .4

STREAM GSTMIN
   SUBSTREAM MIXED TEMP=59 PRES=30
   MASS-FLOW H2O .4

STREAM HI
   SUBSTREAM MIXED TEMP=1736 PRES=362.6
   MASS-FLOW O2 .038 / N2 .99 / CO2 1.041 / H2O .227

STREAM HOTIN
   SUBSTREAM MIXED TEMP=1517.5 PRES=20
   MASS-FLOW TAR .014 / H2 .012 / CO2 .16 / CO .327 /  &
      H2O .51 / CH4 .069 / H2S .001 / NH3 .002 / C2H6  &
      .004 / C2H4 .035 / C2H2 .003

STREAM OFFAIR1
   SUBSTREAM MIXED TEMP=59 PRES=14.696 MASS-FLOW=5
   MOLE-FRAC O2 .207340 / N2 .782180 / CO2 .000330 / H2O  &
      .010150

STREAM OFFFLUE1
   SUBSTREAM MIXED TEMP=1915 PRES=362
   MASS-FLOW O2 .058983 / N2 1.197313 / CO2 1.040337 / CO  &
      .266843

STREAM REFSTMA
   SUBSTREAM MIXED TEMP=59 PRES=30
   MASS-FLOW H2O .544

;

STREAM SAND
   SUBSTREAM MIXED TEMP=1822.0 PRES=25.0
   MASS-FLOW H2O 1.000E-05
   SUBSTREAM CISOLID TEMP=1740.0 PRES=25.0
   MASS-FLOW O2SI 21.0
   SUBSTREAM NC TEMP=1740.0 PRES=25.0
   MASS-FLOW ASH .00780
   COMP-ATTR ASH GENANAL ( 100.0 0.0 0.0 0.0 0.0 0.0 0.0  &
      0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0  &
      0.0 )
   COMP-ATTR ASH ULTANAL ( 100.0 0.0 0. 0.0 0.0 0.0 0.0 )
   COMP-ATTR ASH SULFANAL ( 0.0 0.0 0.0 )
   COMP-ATTR ASH PROXANAL ( 0.0 0.0 0.0 100.0 )

;

STREAM SANDSUPP
   SUBSTREAM MIXED TEMP=59.0 PRES=20
   MASS-FLOW H2O 1.000E-05
   SUBSTREAM CISOLID TEMP=59.0 PRES=20
   MASS-FLOW O2SI .080
```

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;
;=============================================================================
;                              Streams
;=============================================================================
;
;              CoalMisc (8476.0 0.0 0.0 0.0 0.0)

STREAM WOOD
   SUBSTREAM MIXED TEMP=155 PRES=25
   SUBSTREAM CISOLID TEMP=220 PRES=25
   MASS-FLOW CARBON 1.000E-05
   SUBSTREAM NC TEMP=220 PRES=25
   MASS-FLOW WOOD 1.0 / ASH 1.000E-05 / CHAR 1.000E-05
   COMP-ATTR WOOD ULTANAL ( .920 50.880 6.040 .170 .0 .090  &
     41.90 )
   COMP-ATTR WOOD SULFANAL ( .450 .02250 .02250 )
   COMP-ATTR WOOD PROXANAL ( 11.0 15.290 83.520 .870 )
   COMP-ATTR ASH GENANAL ( 100.0 .0 .0 .0 .0 .0 .0 .0  &
     .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 )
   COMP-ATTR ASH ULTANAL ( 100.0 .0 .0 .0 .0 .0 .0 )
   COMP-ATTR ASH SULFANAL ( .0 .0 .0 )
   COMP-ATTR ASH PROXANAL ( .0 .0 .0 100.0 )
   COMP-ATTR CHAR ULTANAL ( .0 86.0 4.0 .0 .0 .030 9.970  &
     )
   COMP-ATTR CHAR SULFANAL ( .010 .010 .010 )
   COMP-ATTR CHAR PROXANAL ( .0 87.180 12.810 .010 )

DEF-STREAMS HEAT 105

DEF-STREAMS HEAT 135

DEF-STREAMS HEAT 197

DEF-STREAMS HEAT 198

DEF-STREAMS HEAT 213

DEF-STREAMS HEAT QAIR

DEF-STREAMS HEAT QCHAR

DEF-STREAMS HEAT QCOMB

DEF-STREAMS HEAT QGAS

DEF-STREAMS HEAT QHT

DEF-STREAMS HEAT QLT

BLOCK B2 MIXER
   PARAM PRES=530

BLOCK DRY1 MIXER
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```
BLOCK DRY2 MIXER

BLOCK DRYRMIX MIXER

;

BLOCK FEEDMIX MIXER
   PARAM PRES=25

BLOCK RECMIX MIXER

BLOCK RECSPLT FSPLIT
   FRAC H2RECYCL .1

BLOCK SANDSPLT FSPLIT
   FRAC SANDPURG .0050

BLOCK B1 SEP
   FRAC STREAM=KOWATER SUBSTREAM=MIXED COMPS=TAR H2 O2 N2  &
      CO2 CO H2O CH4 H2S NH3 COS SO2 SO3 O2SI NO2 NO  &
      PHENOL C6H6 C2H6 C2H4 C2H2 CARBON SULFUR FRACS=0 0  &
      0 0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
   FRAC STREAM=KOWATER SUBSTREAM=CISOLID COMPS=O2SI CARBON  &
      FRACS=0 0
   FRAC STREAM=KOWATER SUBSTREAM=NC COMPS=WOOD ASH CHAR  &
      FRACS=0 0 0

;

BLOCK CHARSEP SEP
   FRAC STREAM=CHAR SUBSTREAM=CISOLID COMPS=O2SI CARBON  &
      FRACS=1.0 1.0
   FRAC STREAM=CHAR SUBSTREAM=NC COMPS=WOOD ASH CHAR FRACS= &
      1.0 1.0 1.0
   FRAC STREAM=SYNGAS SUBSTREAM=MIXED COMPS=TAR H2 O2 N2  &
      CO2 CO H2O CH4 H2S NH3 COS SO2 SO3 O2SI NO2 NO  &
      PHENOL C6H6 C2H6 C2H4 C2H2 CARBON SULFUR FRACS=1.0  &
      1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0  &
      1.0 1.0 1.0 1.0 1.0 1.0 1.0 1.0 0.0 0.0

;

BLOCK COMBSPLT SEP
   FRAC STREAM=ASHSAND SUBSTREAM=MIXED COMPS=TAR H2 O2 N2  &
      CO2 CO H2O CH4 H2S NH3 COS SO2 SO3 O2SI NO2 NO  &
      PHENOL C6H6 C2H6 C2H4 C2H2 CARBON SULFUR FRACS=.0 .0  &
      .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 .0 1.0 .0 .0 .0  &
      .0 .0 .0 .0 .0 .0
   FRAC STREAM=ASHSAND SUBSTREAM=CISOLID COMPS=O2SI FRACS= &
      1.0
   FRAC STREAM=ASHSAND SUBSTREAM=NC COMPS=WOOD ASH CHAR  &
      FRACS=.0 1.0 .0

BLOCK DRYRSEP SEP
```

```
   FRAC STREAM=DRIED SUBSTREAM=MIXED COMPS=TAR H2 O2 N2  &
      CO2 CO H2O CH4 H2S NH3 COS SO2 SO3 O2SI NO2 NO  &
      PHENOL C6H6 C2H6 C2H4 C2H2 CARBON SULFUR FRACS=0 0  &
      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
   FRAC STREAM=DRIED SUBSTREAM=CISOLID COMPS=O2SI CARBON  &
      FRACS=0 0
   FRAC STREAM=DRIED SUBSTREAM=NC COMPS=WOOD ASH CHAR  &
      FRACS=1 0 0

BLOCK PSA SEP
   FRAC STREAM=H2PURIFY SUBSTREAM=MIXED COMPS=TAR H2 O2 N2  &
      CO2 CO H2O CH4 H2S NH3 COS SO2 SO3 O2SI NO2 NO  &
      PHENOL C6H6 C2H6 C2H4 C2H2 CARBON SULFUR FRACS=0 .85  &
      0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
   FRAC STREAM=H2PURIFY SUBSTREAM=CISOLID COMPS=O2SI CARBON  &
      FRACS=0 0
   FRAC STREAM=H2PURIFY SUBSTREAM=NC COMPS=WOOD ASH CHAR  &
      FRACS=0 0 0

BLOCK WOODSEP SEP
   FRAC STREAM=WOODWAT SUBSTREAM=MIXED COMPS=TAR H2 O2 N2  &
      CO2 CO H2O CH4 H2S NH3 COS SO2 SO3 O2SI NO2 NO  &
      PHENOL C6H6 C2H6 C2H4 C2H2 CARBON SULFUR FRACS=1 1  &
      1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
   FRAC STREAM=WOODWAT SUBSTREAM=CISOLID COMPS=O2SI CARBON  &
      FRACS=1 1
   FRAC STREAM=WOODWAT SUBSTREAM=NC COMPS=WOOD ASH CHAR  &
      FRACS=0 1 1

;

BLOCK AIRHEAT HEATER
   PARAM TEMP=60.0 PRES=0

BLOCK B4 HEATER
   PARAM TEMP=190 PRES=0

BLOCK B6 HEATER
   PARAM PRES=0

BLOCK COMBCOOL HEATER
   PARAM PRES=0

BLOCK HTCOOL HEATER
   PARAM TEMP=370 <C> PRES=0

BLOCK REFHTR HEATER
   PARAM TEMP=800 <C> PRES=0

BLOCK REFSTM HEATER
   PARAM TEMP=1000 PRES=0

BLOCK SYNCOOL1 HEATER
   PARAM TEMP=195 PRES=0
```

```
BLOCK STMFLASH FLASH2
   PARAM PRES=130 DUTY=0

BLOCK GSTMGEN HEATX
   PARAM T-COLD=1000 PRES-COLD=0
   FEEDS HOT=SYNREFRM COLD=GSTMIN
   PRODUCTS HOT=FROMPRIM COLD=GASIFSTM

BLOCK INTER2A HEATX
   PARAM T-HOT=150
   FEEDS HOT=GAS2A COLD=160
   PRODUCTS HOT=COOLED2A COLD=STEAM2A

BLOCK INTER2B HEATX
   PARAM T-HOT=150
   FEEDS HOT=GAS2B COLD=165
   PRODUCTS HOT=COOLED2B COLD=STEAM2B

BLOCK LTCOOL HEATX
   PARAM T-HOT=392
   FEEDS HOT=FROMHT COLD=196
   PRODUCTS HOT=TOLT COLD=STEAM6
   FLASH-SPECS TOLT FREE-WATER=YES MAXIT=100
   FLASH-SPECS STEAM6 MAXIT=100

;This block is used to model the syngas cooler prior to compression. Note
;that this block is really only representative of SYNCOOl1 and REFHTR;
;SYNCOOL2 is a separate cooler, modelled by MODEL2.

BLOCK MODEL1 HEATX
   PARAM T-HOT=1472
   FEEDS HOT=HOTIN COLD=COLDIN
   PRODUCTS HOT=HOTOUT COLD=COLDOUT

;This block models the heat exchanger which connects blocks SYNCOOL2
;DECANTHT. SYNCOOL1 is modeled by MODEL1.

BLOCK MODEL2 HEATX
   PARAM T-COLD=1000
   FEEDS HOT=HI COLD=CI
   PRODUCTS HOT=HO COLD=CO

BLOCK PSACOOL HEATX
   PARAM T-HOT=75
   FEEDS HOT=FROMLT COLD=212
   PRODUCTS HOT=TOPSAA COLD=STEAM5
   DECANT-STREA HOT=189
   FLASH-SPECS TOPSAA FREE-WATER=YES

BLOCK STMGEN6 HEATX
   PARAM T-HOT=82
   FEEDS HOT=OFFFLUE2 COLD=188
   PRODUCTS HOT=OFFFLUE3 COLD=STEAM4
```

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;

BLOCK CHARFURN RSTOIC
   PARAM TEMP=1800.0 PRES=-1.0
   STOIC 1 MIXED H2 -1.0 / O2 -.50 / H2O 1.0
   STOIC 2 MIXED O2 -1.0 / CISOLID CARBON -1.0 / MIXED  &
     CO2 1.0
   STOIC 3 MIXED O2 -1.0 / CISOLID SULFUR -1.0 / MIXED  &
     SO2 1.0
   CONV 1 MIXED H2 1.0
   CONV 2 CISOLID CARBON 1.0
   CONV 3 CISOLID SULFUR 1.0

BLOCK HTSHIFT RSTOIC
   PARAM PRES=0 DUTY=0
   STOIC 1 MIXED TAR -1 / H2O -20 / CO2 10 / H2 24
   STOIC 2 MIXED CO -1 / H2O -1 / H2 1 / CO2 1
   CONV 1 MIXED TAR 1
   CONV 2 MIXED CO .7

BLOCK LTSHIFT RSTOIC
   PARAM PRES=0 DUTY=0
   STOIC 1 MIXED CO -1 / H2O -1 / H2 1 / CO2 1
   CONV 1 MIXED CO .75

;

BLOCK GASIFIER RYIELD
   SUBROUTINE YIELD=BATYD
   USER-VECS NREAL=6
   REAL VALUE-LIST=1500.0 360.0 6.60 8.30 .04650 4.0
   PARAM TEMP=1500.0 PRES=20
   BLOCK-OPTION SIM-LEVEL=4

BLOCK OFFCOMB RGIBBS
   PARAM PRES=0

BLOCK PRIMARY RGIBBS
   PARAM TEMP=850 <C> PRES=0 TAPP=-20

BLOCK B3 PUMP
   PARAM PRES=500

BLOCK B5 PUMP
   PARAM PRES=530

BLOCK B7 PUMP
   PARAM PRES=115

BLOCK B13 PUMP
   PARAM PRES=115

BLOCK PUMP1 PUMP
   PARAM PRES=180
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```
BLOCK PUMP4 PUMP
   PARAM PRES=115

BLOCK PUMP5 PUMP
   PARAM PRES=115

BLOCK WATPUMP PUMP
   PARAM PRES=363

BLOCK AIRCOMP1 COMPR
   PARAM TYPE=POLYTROPIC PRES=20

BLOCK AIRCOMP2 COMPR
   PARAM TYPE=POLYTROPIC PRES=19 TEMP=59

BLOCK OFFCOMPR MCOMPR
   PARAM NSTAGE=4 TYPE=POLYTROPIC PRES=362.6
   FEEDS OFFAIR1 1
   PRODUCTS OFFAIR2 4
   COOLER-SPECS 1 TEMP=180 / 2 TEMP=150 / 3 TEMP=150 / 4  &
      TEMP=372.8

BLOCK SYNCOMPR MCOMPR
   PARAM NSTAGE=4 TYPE=POLYTROPIC PRES=530
   FEEDS TOCOMPR 1
   PRODUCTS SYNCOMPD 4 / 205 GLOBAL L
   COOLER-SPECS 1 TEMP=190 / 2 TEMP=190 / 3 TEMP=190 / 4  &
      TEMP=393.1852
   BLOCK-OPTION FREE-WATER=YES

;

BLOCK CHARDEC USER
   DESCRIPTION "CHAR IS DECOMPOSED INTO ITS ELEMENTS"
   SUBROUTINE USRDEC
   BLOCK-OPTION SIM-LEVEL=4

;
;=============================================================================
;                        Design Specifications
;=============================================================================
;

DESIGN-SPEC ADIABAT
   DEFINE GAST INFO-VAR INFO=HEAT VARIABLE=DUTY STREAM=QGAS
   SPEC "GAST" TO "0.D0"
   TOL-SPEC "5."
   VARY BLOCK-VAR BLOCK=GASIFIER VARIABLE=TEMP SENTENCE=PARAM
   LIMITS "1200." "2000."

DESIGN-SPEC AIRTOFLU
   DEFINE WOODT STREAM-VAR STREAM=DRYWOOD SUBSTREAM=MIXED  &
      VARIABLE=TEMP
   SPEC "WOODT" TO "155"
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```
   TOL-SPEC "1.0"
   VARY STREAM-VAR STREAM=DRYRAIR SUBSTREAM=MIXED &
      VARIABLE=MASS-FLOW
   LIMITS "12" "40"

DESIGN-SPEC RECYCLE
   DEFINE H2FRAC MOLE-FRAC STREAM=TOPSAB SUBSTREAM=MIXED &
      COMPONENT=H2
   SPEC "H2FRAC" TO ".7"
   TOL-SPEC ".01"
   VARY BLOCK-VAR BLOCK=RECSPLT SENTENCE=FRAC VARIABLE=FRAC &
      ID1=H2RECYCL
   LIMITS ".1" ".5"

;

DESIGN-SPEC SANDREC
   DEFINE QNONE INFO-VAR INFO=HEAT VARIABLE=DUTY STREAM=QCOMB
   SPEC "QNONE" TO "0.D0"
   TOL-SPEC "10."
   VARY STREAM-VAR STREAM=SANDSUPP SUBSTREAM=CISOLID &
      VARIABLE=MASS-FLOW
   LIMITS "0.01" "40."

DESIGN-SPEC STMGEN6
   DEFINE STMT STREAM-VAR STREAM=STEAM5 SUBSTREAM=MIXED &
      VARIABLE=TEMP
   SPEC "STMT" TO "360"
   TOL-SPEC "1"
   VARY STREAM-VAR STREAM=BFW5 SUBSTREAM=MIXED &
      VARIABLE=MASS-FLOW
   LIMITS ".70" ".85"

DESIGN-SPEC STMGEN8
   DEFINE STMT STREAM-VAR STREAM=STEAM6 SUBSTREAM=MIXED &
      VARIABLE=TEMP
   SPEC "STMT" TO "490"
   TOL-SPEC "1"
   VARY STREAM-VAR STREAM=BFW6 SUBSTREAM=MIXED &
      VARIABLE=MASS-FLOW
   LIMITS ".2" ".3"

FORTRAN COMBAIRT
   DEFINE BLTEMP BLOCK-VAR BLOCK=AIRHEAT VARIABLE=TEMP &
      SENTENCE=PARAM
   DEFINE STRTEM STREAM-VAR STREAM=COMBAIR2 SUBSTREAM=MIXED &
      VARIABLE=TEMP
F    BLTEMP=STRTEM
   EXECUTE AFTER BLOCK AIRCOMP1

;

FORTRAN GASTEMP
   DEFINE TGAS BLOCK-VAR BLOCK=GASIFIER VARIABLE=TEMP &
```

```
      SENTENCE=PARAM
   DEFINE TLIST BLOCK-VAR BLOCK=GASIFIER VARIABLE=VALUE-LIST &
      SENTENCE=REAL ELEMENT=1
F    TLIST = TGAS
F    WRITE(NHSTRY,*) 'WRITE: TLIST = ',TLIST
F    WRITE(NHSTRY,*) 'WRITE: TGAS = ',TGAS
   READ-VARS TGAS
   WRITE-VARS TLIST

FORTRAN OFFAIR
   DEFINE H2 MOLE-FLOW STREAM=OFFGAS SUBSTREAM=MIXED &
      COMPONENT=H2
   DEFINE CO MOLE-FLOW STREAM=OFFGAS SUBSTREAM=MIXED &
      COMPONENT=CO
   DEFINE CH4 MOLE-FLOW STREAM=OFFGAS SUBSTREAM=MIXED &
      COMPONENT=CH4
   DEFINE C2H6 MOLE-FLOW STREAM=OFFGAS SUBSTREAM=MIXED &
      COMPONENT=C2H6
   DEFINE C2H4 MOLE-FLOW STREAM=OFFGAS SUBSTREAM=MIXED &
      COMPONENT=C2H4
   DEFINE C2H2 MOLE-FLOW STREAM=OFFGAS SUBSTREAM=MIXED &
      COMPONENT=C2H2
   DEFINE AIRFLO STREAM-VAR STREAM=OFFAIR1 SUBSTREAM=MIXED &
      VARIABLE=MOLE-FLOW
   DEFINE O2FRAC MOLE-FRAC STREAM=OFFAIR1 SUBSTREAM=MIXED &
      COMPONENT=O2
F    O2MOL=(.5*H2+.5*CO+2*CH4+3.5*C2H6+3*C2H4+2.5*C2H2)
F    AIRFLO=1.15*O2MOL/O2FRAC
   EXECUTE BEFORE BLOCK OFFCOMB

FORTRAN PRESDROP
   DEFINE P1 STREAM-VAR STREAM=SYNCOMPD SUBSTREAM=MIXED &
      VARIABLE=PRES
   DEFINE HTPRES BLOCK-VAR BLOCK=HTSHIFT VARIABLE=PRES &
      SENTENCE=PARAM
   DEFINE LTPRES BLOCK-VAR BLOCK=LTSHIFT VARIABLE=PRES &
      SENTENCE=PARAM
   DEFINE PRIMP BLOCK-VAR BLOCK=PRIMARY VARIABLE=PRES &
      SENTENCE=PARAM
F    PRIMP = 0.95 * P1
F    HTPRES = 0.85 * PRIMP
F    LTPRES = 0.85 * HTPRES
   EXECUTE AFTER BLOCK PRIMARY

FORTRAN REFSTM
   DEFINE STM MOLE-FLOW STREAM=REFSTMA SUBSTREAM=MIXED &
      COMPONENT=H2O
   DEFINE TAR MOLE-FLOW STREAM=TOREFHOT SUBSTREAM=MIXED &
      COMPONENT=TAR
   DEFINE CO MOLE-FLOW STREAM=TOREFHOT SUBSTREAM=MIXED &
      COMPONENT=CO
   DEFINE CH4 MOLE-FLOW STREAM=TOREFHOT SUBSTREAM=MIXED &
      COMPONENT=CH4
   DEFINE C2H6 MOLE-FLOW STREAM=TOREFHOT SUBSTREAM=MIXED &
```

```
      COMPONENT=C2H6
    DEFINE C2H4 MOLE-FLOW STREAM=TOREFHOT SUBSTREAM=MIXED &
      COMPONENT=C2H4
    DEFINE C2H2 MOLE-FLOW STREAM=TOREFHOT SUBSTREAM=MIXED &
      COMPONENT=C2H2
    DEFINE EXIST MOLE-FLOW STREAM=TOREFHOT SUBSTREAM=MIXED &
      COMPONENT=H2O
F   STM=3*(10*TAR+CO+1*CH4+2*C2H6+2*C2H4+2*C2H2)-EXIST
    EXECUTE BEFORE BLOCK PRIMARY

FORTRAN SETCSEP
    DEFINE TEMPIN STREAM-VAR STREAM=WOODGAS SUBSTREAM=MIXED &
      VARIABLE=TEMP
    DEFINE TSEP BLOCK-VAR BLOCK=CHARSEP VARIABLE=TEMP &
      SENTENCE=FLASH-SPECS ID1=CHAR
    DEFINE TSEPG BLOCK-VAR BLOCK=CHARSEP VARIABLE=TEMP &
      SENTENCE=FLASH-SPECS ID1=SYNGAS
F   TSEP  = TEMPIN
F   TSEPG = TEMPIN
    READ-VARS TEMPIN
    WRITE-VARS TSEP TSEPG

;

FORTRAN STEAMAMT
    DEFINE STEAM MASS-FLOW STREAM=GASIFSTM SUBSTREAM=MIXED &
      COMPONENT=H2O
    DEFINE WOOD MASS-FLOW STREAM=WOOD SUBSTREAM=NC &
      COMPONENT=WOOD
F   STEAM = 0.4 * WOOD
    READ-VARS WOOD
    WRITE-VARS STEAM

FORTRAN WOODDRY
    DEFINE REALNC STREAM-VAR STREAM=WOOD SUBSTREAM=NC &
      VARIABLE=MASS-FLOW
    DEFINE REALMI STREAM-VAR STREAM=WOOD SUBSTREAM=MIXED &
      VARIABLE=MASS-FLOW
    DEFINE REALCI STREAM-VAR STREAM=WOOD SUBSTREAM=CISOLID &
      VARIABLE=MASS-FLOW
    DEFINE NEWNC STREAM-VAR STREAM=ARWOOD SUBSTREAM=NC &
      VARIABLE=MASS-FLOW
    DEFINE NEWMIX STREAM-VAR STREAM=ARWOOD SUBSTREAM=MIXED &
      VARIABLE=MASS-FLOW
    DEFINE NEWCI STREAM-VAR STREAM=ARWOOD SUBSTREAM=CISOLID &
      VARIABLE=MASS-FLOW
    DEFINE NEWH2O MASS-FLOW STREAM=ARWOOD SUBSTREAM=MIXED &
      COMPONENT=H2O
F   NEWNC = REALNC
F   NEWH2O = 0.78 * REALNC
F   NEWMIX = REALMI + NEWH2O
F   NEWCI = REALCI
    EXECUTE BEFORE BLOCK WOODSEP
```

```
;

FORTRAN XSAIR
   DEFINE PCARB MOLE-FLOW STREAM=CHARCOMP SUBSTREAM=CISOLID  &
      COMPONENT=CARBON
   DEFINE PHYDRO MOLE-FLOW STREAM=CHARCOMP SUBSTREAM=MIXED  &
      COMPONENT=H2
   DEFINE PSULF MOLE-FLOW STREAM=CHARCOMP SUBSTREAM=CISOLID  &
      COMPONENT=SULFUR
   DEFINE AIRFLO STREAM-VAR STREAM=COMBAIR SUBSTREAM=MIXED  &
      VARIABLE=MOLE-FLOW
   DEFINE O2FRAC MOLE-FRAC STREAM=COMBAIR SUBSTREAM=MIXED  &
      COMPONENT=O2
F     O2MOL = PCARB + 0.5*PHYDRO + PSULF
F     AIRFLO = 1.2 * O2MOL / O2FRAC
   READ-VARS PCARB PHYDRO PSULF O2FRAC
   WRITE-VARS AIRFLO

CONV-OPTIONS
   PARAM CHECKSEQ=NO

CONVERGENCE C-GASSTM WEGSTEIN
   TEAR GASIFSTM

CONVERGENCE C-H2REC WEGSTEIN
   TEAR H2RECYCL

CONVERGENCE C-SAND WEGSTEIN
   TEAR SAND .0010
   PARAM MAXIT=50 QMIN=-5.0

CONVERGENCE MIXTEAR WEGSTEIN
   TEAR 207

CONVERGENCE C-AIRFLU SECANT
   SPEC AIRTOFLU

;

CONVERGENCE C-QGAS SECANT
   SPEC ADIABAT

CONVERGENCE C-SANDR SECANT
   SPEC SANDREC

CONVERGENCE H2SPLT SECANT
   SPEC RECYCLE

CONVERGENCE STMGEN6 SECANT
   SPEC STMGEN6

CONVERGENCE STMGEN8 SECANT
   SPEC STMGEN8
```

```
SEQUENCE S-1 STEAMAMT C-GASSTM C-SAND FEEDMIX C-QGAS GASTEMP &
     GASIFIER (RETURN C-QGAS) SETCSEP CHARSEP CHARDEC XSAIR &
     AIRCOMP1 COMBAIRT AIRHEAT C-SANDR CHARFURN &
     (RETURN C-SANDR) COMBSPLT SANDSPLT (RETURN C-SAND) &
     SYNCOOL1 MIXTEAR B1 B5 SYNCOMPR B2 (RETURN MIXTEAR) &
     REFHTR REFSTM WATPUMP REFSTM PRESDROP PRIMARY GSTMGEN &
     (RETURN C-GASSTM) C-AIRFLU AIRCOMP2 DRYRMIX WOODDRY &
     WOODSEP DRY1 DRY2 DRYRSEP (RETURN C-AIRFLU) HTCOOL &
     HTSHIFT STMGEN8 B3 LTCOOL (RETURN STMGEN8) LTSHIFT B7 &
     PSACOOL H2SPLT C-H2REC RECMIX PSA RECSPLT &
     (RETURN C-H2REC) (RETURN H2SPLT) OFFAIR OFFCOMPR OFFCOMB &
     COMBCOOL B13 STMGEN6 MODEL1 MODEL2 PUMP1 B4 B6 &
     STMFLASH PUMP4 INTER2A PUMP5 INTER2B

STREAM-REPOR ZEROFLOW MOLEFLOW MASSFLOW MOLEFRAC MASSFRAC &
     NOCOMP-ATTR

PROPERTY-REP NOPARAMS

REPORT-SCALE
   DEFINE WOOD STREAM-VAR STREAM=WOOD SUBSTREAM=NC &
     VARIABLE=MASS-FLOW
   SCALE "WOOD" TO "1"

PROP-TABLE PT-1 PROPS
   STREAM COMBAIR
   VARY TEMP
   RANGE LOWER=100.0 UPPER=2400.0 INCR=100.0
   TABULATE "PROPERTIES TABLE FOR CONV. COMPS" PROPERTIES=PS-1

PROP-TABLE PT-2 PROPS
   STREAM WOOD
   VARY TEMP
   RANGE LOWER=100.0 UPPER=2400.0 INCR=100.0
   TABULATE "PROPS FOR NC COMPS" PROPERTIES=PS-2
```

```
C$ #2 BY: MKMANN  6/08/94 MODIFIED TO MODEL THE BATTELLE GASIFIER
C$ #1 BY: KRCRAIG 5/21/93 NEW
C
C-------------------------------------------------------------------
C                   **** NOTICE ****
C-------------------------------------------------------------------
C
C
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%
C
C        THIS CODE IS PART OF THE SYSTEM DEVELOPED AT
C     NATIONAL RENEWABLE ENERGY LABORATORY, GOLDEN, COLORADO
C
C
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%
C
C
      SUBROUTINE BATYD (SIN ,SOUT , NSUBS,IDXSUB,ITYPE,NINT,INT,NREAL,
     1                 REAL,IDS,NPO,NBOPST,NIW,IW,NW,W)
C
C
C  NAME OF MODULE: USRDEV
C
C  MODULE TITLE: WOOD DEVOLATILIZATION AND PYROLYSIS
C
C  PURPOSE: USER ROUTINE TO MODEL FIXED-BED GASIFICATION WOOD
C         DEVOLATILIZATION BASED ON THE ULTIMATE ANALYSIS OF
C         THE WOOD, TAR, OIL, NAPHTHA, PHENOL, AND CHAR.
C
C  WRITTEN BY:  K. R. CRAIG              DATE WRITTEN:  5/21/93
C
C  BASED ON NYLD ROUTINE WRITTEN BY M.I.T. FOR CONOCO STUDY (12/15/81)
C
C
C    VARIABLES IN ARGUMENT LIST
C
C    VAR   I/O  TYPE   DIM     DESCRIPTION
C
C    SIN     I/O   R           INLET MATERIAL STREAM VECTOR
C    SOUT     O    R           OUTLET MATERIAL STREAM VECTOR
C    NSUBS   I    I            NUMBER OF SUBSTREAMS
C    IDXSUB  I    I    NSUBS   SUBSTREAM INDEX VECTOR
C    ITYPE   I    I    NSUBS   SUBSTREAM TYPE VECTOR
C    NINT    I    I            LENGTH OF INTEGER VECTOR
C    INT     I/O  I    NINT    INTEGER VECTOR
C    NREAL   I    I            LENGTH OF REAL VECTOR
C    REAL    I    R    NREAL   REAL ARRAY
C    REAL(1) I    R            OUTLET TEMPERATURE
C    REAL(2) I    R            OUTLET PRESSURE
C    IDS     I    I    2,NCC   ID VECTOR
C    NPO     I    I            NUMBER OF PHYSICAL PROPERTY OPTIONS
C    NBOPST  I    I    3,NPO   PHYSICAL PROPERTY OPTION SET POINTERS
```

```
C   NIW    I  I          LENGTH OF THE INTEGER WORK VECTOR
C   IW     I  I   NIW    INTEGER WORK VECTOR
C   NW     I  I          LENGTH OF THE REAL WORK VECTOR
C   W      I  R   NW     REAL WORK VECTOR
C
C
C    IMPORTANT INTERNAL VARIABLES
C
C   VAR    TYPE  DIM   DESCRIPTION
C
C   HYDCAR  R     6    HYDROCARBON YIELD FROM DRY ASH-FREE WOOD
C                      HYDCAR(1) = TAR
C                      HYDCAR(2) = PHENOL
C                      HYDCAR(3) = NAPHTHA
C                      HYDCAR(4) = OIL
C                      HYDCAR(5) = CHAR
C                      HYDCAR(6) = C2H6
C   SDIST   R     3    DISTRIBUTION OF SULFUR COMPOUNDS (SUM=1.0)
C                      SDIST(1) = H2S
C                      SDIST(2) = COS
C                      SDIST(3) = CS2
C   RNDIST  R     2    DISTRIBUTION OF NITROGEN COMPOUNDS (SUM=1.0)
C                      RNDIST(1) = NH3
C                      RNDIST(2) = N2
C   IDX     I    99    COMPONENT INDEX VECTOR
C   X       R    99    COMPONENT MOLAR FRACTION VECTOR
C   L1      I          POINTER TO MIXED SUBSTREAM
C   L2      I          POINTER TO CISOLID SUBSTREAM
C   L3      I          POINTER TO NC SUBSTREAM
C
C
C  ERROR CONDITIONS:
C
C   NUMBER  LEVEL
C
C   8600000  0
C
C   IMPROPER STREAM STRUCTURE.
C   STREAM STRUCTURE MUST BE MIXED + CISOLID + NC, IN THAT ORDER.
C
C   8600001  1
C
C   ULTIMATE ANALYSIS IS MISSING FOR ONE OR MORE OF THESE COMPONENTS:
C     TAR, OIL, PHENOL, NAPHTHA, CHAR.
C
C   8600002  2
C
C   ULTANAL MUST NOT CONTAIN CHLORINE.  MASS BALANCE WILL BE IN ERROR.
C
C
C  SUBROUTINES CALLED:
C
C   NAME - LOCATI (FUNCTION)
C   DESC - INTEGER BEAD LOCATOR
```

```
C
C     NAME - LOCATS
C     DESC - STREAM BEAD LOCATOR
C
C     NAME - APSCPY
C     DESC - STREAM COPIER
C
C     NAME - UCONV1
C     DESC - CONVERTS VALUE TO SI UNITS
C
C     NAME - NSQCC
C     DESC - FINDS SEQUENCE NUMBER OF A CONVENTIONAL COMPONENT
C
C     NAME - NSQNCC
C     DESC - FINDS SEQUENCE NUMBER OF A NONCONVENTIONAL COMPONENT
C
C     NAME - CPACK
C     DESC - CONVENTIONAL PHASES PACKING
C
C     NAME - AVEMW (FUNCTION)
C     DESC - AVERAGE SUBSTREAM MOLECULAR WEIGHT
C
C     NAME - TOTENT
C     DESC - TOTAL STREAM ENTHALPY
C
C     NAME - FLASH
C     DESC - GENERAL PURPOSE FLASH INTERFACE ROUTINE
C
C     NAME - MERRPT (FUNCTION)
C     DESC - ERROR MESSAGE CHECKING
C
C     NAME - ERROR
C     DESC - ERROR HANDLING ROUTINE
C
C
C   USING THIS MODEL:
C
C     WOOD, CHAR, TAR, OIL, PHENOL, AND NAPHTHA ARE EXPECTED TO HAVE
C     ULTIMATE ANALYSES.  ANY CHLORINE IN THE ULTIMATE ANALYSES WILL
C     BE IGNORED, RESULTING IN A MASS BALANCE ERROR.  TAR, OIL, PHENOL,
C     AND NAPHTHA SHOULD BE IN THE MIXED SUBSTREAM.  THE ASSUMED STREAM
C     STRUCTURE IS MIXED + CISOLID + NC.
C
C
C     ***************************************************
C     *                                                 *
C     *    THE COMPONENTS LISTED BELOW ARE REQUIRED.    *
C     *       ALL OTHERS ARE CONSIDERED INERT.          *
C     *                                                 *
C     *            WOOD       CO                      *
C     *            ASH        H2                      *
C     *            CHAR       N2                      *
C     *            CARBON     H2O                     *
C     *            TAR        H2S                     *
```

```
C    *            OIL       CS2              *
C    *            PHENOL    COS                *
C    *            NAPHTHA   NH3                 *
C    *                  C2H6               *
C    *                                   *
C    ***************************************************
C
C
C  DECLARATIONS & COMMONS
C
      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION SIN(1), SOUT(1), IDXSUB(NSUBS), ITYPE(NSUBS),
     1          INT(NINT), REAL(NREAL), NBOPST(3,NPO),
     2          IW(NIW), W(NW), IDS(2,12)
      DIMENSION RETN(337),IRETN(6)
      DIMENSION IPROG(2)
      DIMENSION ITAR(2),IOIL(2),IPHNOL(2),INAPTH(2),ICHAR(2),IWOOD(2),
     1          IH2S(2),INH3(2),ICARBN(2),ICOS(2),ICO(2),IH2(2),
     2          IN2(2),IC2H6(2),IASH(2),ICS2(2),IH2O(2),IC2H4(2),
     3          IC6H6(2),IO2(2),ICH4(2),ICO2(2), IC2H2(2)
      DIMENSION IDX(99),X(99)
      DIMENSION XH2(3),XCO(3),XCO2(3),XCH4(3),XC2H2(3),XC2H4(3),
     1          XC2H6(3),XC6H6(3),XCHAR(3),XTAR(2),XDGAS(3)
      COMMON /USER/   RMISS, IMISS, NGBAL, IPASS, IRESTR, ICONVG, LMSG,
     1               LPMSG, KFLAG, NHSTRY, NRPT, NTRMNL
      COMMON /NCOMP/  NCC, NNCC
      DIMENSION B(1)
      EQUIVALENCE (IB(1), B(1))
      INTEGER XMW
      COMMON / IPOFF1 / IPOFF1(1)
      COMMON /RGLOB/  DUMMY1, RMIN
C     INTEGER IDXCC
      COMMON / IPOFF8 / IPOFF8(1)
      INTEGER IDXNCC
      INTEGER IPROX
      COMMON / IPOFF2 / IPOFF2(1)
      INTEGER IULT
      COMMON /PLEX/   IB(1)
C
C  DATA STATEMENTS
C
      DATA IPROG /4HBATY,4HD   /
      DATA ITAR/4HTAR ,4H    /,IOIL/4HOIL ,4H    /,IPHNOL/4HPHEN,4HOL  /
     1,INAPTH/4HNAPH,4HTHA /,ICHAR /4HCHAR,4H    /,IWOOD /4HWOOD,4H    /
     2,ICARBN/4HCARB,4HON  /,ICOS  /4HCOS ,4H    /,IH2S  /4HH2S ,4H    /
     3,INH3  /4HNH3 ,4H    /,ICO   /4HCO  ,4H    /
     4,IH2   /4HH2  ,4H    /,IN2   /4HN2  ,4H    /,IC2H6 /4HC2H6,4H    /
     5,IASH  /4HASH ,4H    /,ICS2  /4HCS2 ,4H    /,IH2O  /4HH2O ,4H    /
     6,IO2   /'O2  ','     '/,IC2H4 /'C2H4','    '/,IC6H6 /'C6H6','    '/
     7,ICH4  /'CH4 ','     '/,IC2H2 /'C2H2','    '/
     8,ICO2  /'CO2 ','     '/
C
      DATA XDGAS / 2.8993D+01, -4.3325D-02, 2.0966D-05  /
     2,    XCO / 133.46, -0.10290, 2.8792D-5  /
```

```
     4,   XCO2 / -9.5251, 0.037889, -1.4927D-5  /
     6,   XCH4/  -13.82, 0.044179, -1.6167D-5  /
     8,   XC2H4/ -38.258, 0.058435, -1.9868D-5  /
     1,   XC2H6/ 11.114, -0.011667, 3.064D-6  /
     3,   XH2 / 17.996, -0.026448, 1.8930D-5  /
     9,   XC2H2 / -4.3114, 5.4499D-3, -1.561D-6 /
     5,   XCHAR/ 0.75503, -3.0212D-4, -3.1178D-8  /
     7,   XTAR/ 0.045494, -1.9759D-5  /
C
C  CHECK FOR REPORT PASS
C
C
C  STATEMENT FUNCTIONS FOLLOW
C
      XMW(I) = LMW + I
C       IDXCC(I) = LIDXC + I
      IDXNCC(I) = LIDXN + I
      IPROX(I) = LPRXA + I
      IULT(I) = LULTA + I
C
C  SET PLEX OFFSETS
C
      LMW = IPOFF1(306)
      LIDXC = IPOFF8(4)
      LIDXN = IPOFF8(5)
      LPRXA = IPOFF2(10)
      LULTA = IPOFF2(12)
      IF (IPASS.EQ.4) RETURN
C
C INITIALIZE VARIABLES AND POINTERS
C
      IULTTR = 0
      IULT0I = 0
      IULTPH = 0
      IULTNA = 0
      IULTCH = 0
      IPRXWD = 0
      IPRXCH = 0
      IULTWD = 0
C
C  COPY INLET STREAM INTO OUTLET STREAM
C
C  LOCATE BLOCK BEAD
      LPROC = LOCATI(2)
      LBSMB = LOCATI(IB(LPROC+3))
      LBLK = IB(LBSMB+5)
C  LOCATE STREAM BEADS
      NBSIN  = IB(LBLK + IB(LBLK+17))
      NBSOUT = IB(LBLK + IB(LBLK+19))
      CALL LOCATS(NBSIN,LVI1,LVR1,LD,NBD)
      CALL LOCATS(NBSOUT,LVI2,LVR2,LD,NBD)
C  COPY THE STREAM
      CALL APSCPY(LD,LVR1,LVR2)
C
```

```
C  CHECK FOR IMPROPER STREAM STRUCTURE
C
      IF (NSUBS.NE.3) GOTO 820
      IF (ITYPE(1).NE.1 .OR. ITYPE(2).NE.2 .OR. ITYPE(3).NE.3) GOTO 820
C
C  SET OUTLET TEMPERATURE AND PRESSURE (IN SI UNITS)
C
      TOUTF= REAL(1)
      TOUT = REAL(1)
      POUT = REAL(2)
      CALL UCONV1(22,TOUT)
      CALL UCONV1(20,POUT)
      IF (POUT.LE.0.0) POUT=SIN(NNCC+3)+POUT
C
C  FIND COMPONENT INDEX NUMBERS
C
      CALL NSQCC(ITAR,NTAR)
C       CALL NSQCC(IOIL,NOIL)
C       CALL NSQCC(IPHNOL,NPHNOL)
C       CALL NSQCC(INAPTH,NNAPTH)
      CALL NSQCC(ICARBN,NCARBN)
C       CALL NSQCC(ICOS,NCOS)
C       CALL NSQCC(ICS2,NCS2)
      CALL NSQCC(IH2S,NH2S)
      CALL NSQCC(IH2O,NH2O)
      CALL NSQCC(INH3,NNH3)
      CALL NSQCC(ICO,NCO)
      CALL NSQCC(ICO2,NCO2)
      CALL NSQCC(IH2,NH2)
      CALL NSQCC(IN2,NN2)
      CALL NSQCC(IO2,NO2)
      CALL NSQCC(IC2H6,NC2H6)
      CALL NSQCC(IC2H4,NC2H4)
      CALL NSQCC(IC2H2,NC2H2)
      CALL NSQCC(IC6H6,NC6H6)
      CALL NSQCC(ICH4,NCH4)
      CALL NSQNCC(IWOOD,NWOOD)
      CALL NSQNCC(IASH,NASH)
      CALL NSQNCC(ICHAR,NCHAR)
C
C  ATOMIC (NOT MOLECULAR) WEIGHTS FOR CARBON, HYDROGEN, NITROGEN,
C  SULFUR, AND OXYGEN.
C
      CAW  = B(XMW(NCARBN))
      HAW  = B(XMW(NH2))/2
      RNAW = B(XMW(NN2))/2
      SAW  = 32.064
      OAW  = 16.0
C
C  FIND OUT WHERE ATTRIBUTES ARE STORED FOR ATTRIBUTED COMPONENTS.
C
      DO 150 I=1,NSUBS
        ILOC = ITYPE(I)
        NCT = NCC
```

```
      IF (ILOC .EQ. 3) NCT = NNCC
      IATLST = IDXSUB(I) + NCT + 8
      GOTO (120,130,140), ILOC
  120 CONTINUE
      L1 = IDXSUB(I) - 1
C       IULTTR = IATLST + IULT(IDXCC(NTAR))
C       IULTOI = IATLST + IULT(IDXCC(NOIL))
C       IULTPH = IATLST + IULT(IDXCC(NPHNOL))
C       IULTNA = IATLST + IULT(IDXCC(NNAPTH))
      GOTO 150
  130 CONTINUE
      L2 = IDXSUB(I) - 1
      GOTO 150
  140 CONTINUE
      L3 = IDXSUB(I) - 1
      IULTCH = IATLST + IB(IULT(IB(IDXNCC(NCHAR))))
      IPRXWD = IATLST + IB(IPROX(IB(IDXNCC(NWOOD))))
      IPRXCH = IATLST + IB(IPROX(IB(IDXNCC(NCHAR))))
      IULTWD = IATLST + IB(IULT(IB(IDXNCC(NWOOD))))
      TOTAL = SIN(L3 + NWOOD)
  150 CONTINUE
C
C     CHKSUM = IULTTR + IULTOI + IULTPH + IULTNA + IULTCH
     CHKSUM = IULTCH
     IF (CHKSUM.LT.RMISS) GOTO 170
     ISEV=1
     IF (MERRPT(IPROG,IDS,ISEV,8600001,LMSG,KFLAG).NE.0)
    &  WRITE(NHSTRY,160)
  160 FORMAT(6X,'ULTIMATE ANALYSIS IS MISSING FOR ONE OR MORE OF '
    &  'THESE COMPONENTS:'/9X'TAR, OIL, PHENOL, NAPHTHA, CHAR.')
C     CALL ERRSP(ISEV,3)
  170 CONTINUE
C
C     CHKSUM = SIN(IULTTR+5) + SIN(IULTOI+5) + SIN(IULTPH+5)
C    &      + SIN(IULTNA+5) + SIN(IULTCH+5)
     CHKSUM =  SIN(IULTCH+5)
     IF (CHKSUM.LT.RMIN) GOTO 190
     ISEV=2
     IF (MERRPT(IPROG,IDS,ISEV,8600002,LMSG,KFLAG).NE.0)
    &  WRITE(NHSTRY,180)
  180 FORMAT(6X,'ULTANAL MUST NOT CONTAIN CHLORINE.  MASS BALANCE '
    &  'WILL BE IN ERROR.')
C     CALL ERRSP(ISEV,3)
  190 CONTINUE
C
C  GET MOISTURE CONTENT OF WOOD. GET DRY WEIGHT OF WOOD.
C
     WATER = SIN(IPRXWD+1)*TOTAL/100.
     BDW = TOTAL - WATER
     H2O = WATER / B(XMW(NH2O))
     TMULT = BDW/100.
     write(nhstry,992) total,water,(sin(iultwd+i),i=1,7),caw,haw,
    &                  rnaw,saw,oaw
  992 format(/,' wood flow=',g12.5,  ' moisture=',g12.5,
```

```
     1       ' ash %='    ,g12.5,/,' carb%='   ,g12.5,
     2       ' hyd%='     ,g12.5,  ' nitr%=',   g12.5,
     3      /,' cl%='      ,g12.5,  ' sulf%='   ,g12.5,
     4       ' oxygen%='  ,g12.5,/,' caw='     ,g12.5,
     5       ' haw= '     ,g12.5,  ' rnaw= '   ,g12.5,
     6      /,' saw= '     ,g12.5,  ' oaw= '    ,g12.5,/)
C
C  GET INDIVIDUAL ELEMENT TOTAL FLOWS
C
C            SANDIN = SIN(L2+NO2SI)
C            SANDOUT = SOUT(L2+NO2SI)
C            SANDDIF = SANDOUT-SANDIN
      TASH  = SIN(IULTWD+1) * TMULT
      TCARB = SIN(IULTWD+2) * TMULT / CAW
      THYD  = SIN(IULTWD+3) * TMULT / HAW
      TRNIT = SIN(IULTWD+4) * TMULT / RNAW
      TSULF = SIN(IULTWD+6) * TMULT / SAW
      TOXY  = SIN(IULTWD+7) * TMULT / OAW
      WRITE(NHSTRY,999) TASH,TCARB,THYD,TRNIT,TSULF,TOXY
  999 FORMAT(/,' WRITE: WOOD ELEMENTS',/
     1       ' MOLES OF ATOMS',/,' ASH ',G12.5,' CARBON ',G12.5,
     2       ' HYDROGEN ',G12.5,/,' NITROGEN ',G12.5,' SULFUR ',
     3       G12.5,' OXYGEN ',G12.5)
C
C  YIELD OF HYDROCARBONS BASED ON A MOISTURE AND ASH FREE BASIS
C  DGAS AND GAS COMPONENTS IN SCF (59 F, 1 ATM)
C  CHAR AND TAR IN LB

      ZMAF = BDW - TASH
C        ZMAF = MOISTURE AND ASH FREE WOOD (KG/SEC)
      WRITE(NHSTRY,*) 'ZMAF = ',ZMAF
      ZLBMAF = ZMAF*2.20462*3600
C        ZLBMAF = MOISTURE AND ASH FREE WOOD (LB/HR)
      WRITE(NHSTRY,*) 'ZLBMAF = ',ZLBMAF
      ZLBBDW = BDW * 2.20462 *3600
      WRITE(NHSTRY,*) 'ZLBBDW = ',ZLBBDW
      T2 = TOUTF**2
      T1 = TOUTF
      WRITE(NHSTRY,*) 'TOUT = ',TOUT
      WRITE(NHSTRY,*) 'T1 = ',T1
      WRITE(NHSTRY,*) 'T2 = ',T2
      DGAS = (XDGAS(1) + T1*XDGAS(2) + T2*XDGAS(3)) * ZLBMAF
      WRITE(NHSTRY,*) 'DGAS IN SCF = ',DGAS
      WRITE(NHSTRY,*) 'MAF IN LB = ',ZLBMAF
      H2 = (XH2(1) + T1*XH2(2) + T2*XH2(3)) * DGAS/100
      write(nhstry,*) ' WRITE: bdw= ',bdw,' h2= ',h2, ' DGAS= ',DGAS
      CO =  (XCO(1) + T1*XCO(2) + T2*XCO(3)) * DGAS/100
      write(nhstry,*) ' WRITE: CO(scf)=',CO
      CO2 = (XCO2(1) + T1*XCO2(2) + T2*XCO2(3)) * DGAS/100
      write(nhstry,*) ' WRITE: CO2(scf)=',CO2
      CH4 = (XCH4(1) + T1*XCH4(2) + T2*XCH4(3)) * DGAS/100
      write(nhstry,*) ' WRITE: CH4(scf)=',CH4
      C2H2 = (XC2H2(1) + T1*XC2H2(2) + T2*XC2H2(3)) * DGAS/100
      write(nhstry,*) ' WRITE: C2H2(scf)=',C2H2
```

```
      C2H4 = (XC2H4(1) + T1*XC2H4(2) + T2*XC2H4(3)) * DGAS/100
      write(nhstry,*) ' WRITE: C2H4(scf)=',C2H4
      C2H6 = (XC2H6(1) + T1*XC2H6(2) + T2*XC2H6(3)) * DGAS/100
      write(nhstry,*) ' WRITE: C2H6(scf)=',C2H6
      CHAR = (XCHAR(1) + T1*XCHAR(2) + T2*XCHAR(3)) * ZLBBDW
      WRITE(NHSTRY,*) 'WRITE: CHAR (LB) = ',CHAR
      TAR = (XTAR(1) + T1*XTAR(2)) * ZLBBDW
      write(nhstry,*) ' WRITE: TAR(LB)=',TAR

C  CONVERT PRODUCT GAS FLOWS IN SCF AND TAR AND CHAR IN LB TO MOLAR BASI

      H2MOL = H2 / 379.4630 / 2.20462 / 3600
      write(nhstry,*) ' WRITE: mwh2= ',B(xmw(nh2)),' h2mol= ',h2mol
      COMOL = CO / 379.4630 / 2.20462 / 3600
      write(nhstry,*) ' WRITE: mwCO= ',B(xmw(nCO)),' COmol= ',COmol
      CO2MOL = CO2 / 379.4630 / 2.20462 / 3600
      write(nhstry,*) ' WRITE: mwCO2 = ',B(xmw(nCO2)),' CO2mol= ',CO2mol
      CH4MOL = CH4 / 379.4630 / 2.20462 / 3600
      write(nhstry,*) ' WRITE: mwCH4 = ',B(xmw(nCH4)),' CH4mol= ',CH4mol
      C2H2MOL = C2H2 / 379.4630 / 2.20462 / 3600
      C2H4MOL = C2H4 / 379.4630 / 2.20462 / 3600
      C2H6MOL = C2H6 / 379.4630 / 2.20462 / 3600
C     C6H6MOL = C6H6 / 379.4630 / 2.20462 / 3600
      TARMOL = TAR/B(XMW(NTAR)) / 2.20462 / 3600
      write(nhstry,*) ' WRITE: mwTAR = ',B(xmw(nTAR)),' TARmol= ',TARmol
      if (h2mol .lt. 0.d0) h2mol = 0.d0
      if (h2mol .lt. 0.d0) WRITE(NHSTRY,*) ' WRITE: H2MOL = 0 (407)'
      if (comol .lt. 0.d0) comol = 0.d0
      if (comol .lt. 0.d0) WRITE(NHSTRY,*) ' WRITE: COMOL = 0 (409) '
      if (co2mol .lt. 0.d0) co2mol = 0.d0
      if (co2mol .lt. 0.d0) WRITE(NHSTRY,*) ' WRITE: CO2MOL = 0 (411) '
      if (ch4mol .lt. 0.d0) ch4mol = 0.d0
      if (ch4mol .lt. 0.d0) WRITE(NHSTRY,*) 'WRITE: CH4MOL = 0 (413) '
      if (c2h4mol .lt. 0.d0) c2h4mol = 0.d0
      if (c2h4mol .lt. 0.d0) WRITE(NHSTRY,*) 'WRITE: CH24MOL = 0 (415) '
      if (c2h2mol .lt. 0.d0) c2h2mol = 0.d0
      if (c2h2mol .lt. 0.d0) WRITE(NHSTRY,*) 'WRITE: C2H2MOL = 0 (415) '
      if (c2h6mol .lt. 0.d0) c2h6mol = 0.d0
      if (c2h6mol .lt. 0.d0) WRITE(NHSTRY,*) 'WRITE: C2H6MOL = 0 (417) '
C     if (c6h6mol .lt. 0.d0) c6h6mol = 0.d0
C     if (c6h6mol .lt. 0.d0) WRITE(NHSTRY,*) 'WRITE: C6H6MOL = 0 (419) '
      if (TARmol .lt. 0.d0) TARmol = 0.d0
      if (TARmol .lt. 0.d0) WRITE(NHSTRY,*) 'WRITE: TARMOL = 0 (421) '
      WRITE(NHSTRY,998)H2MOL,COMOL,CO2MOL,CH4MOL,C2H4MOL,
     1                 C2H6MOL,TARMOL
  998 FORMAT(/,' GASIF. PRODUCTS',/
     1       ' MOLES ',/,' H2  ',G12.5,' CO   ',G12.5,
     2       ' CO2  ',G12.5,/,' CH4 ',G12.5,' C2H4 ',
     3       G12.5,' C2H6 ',G12.5,G12.5,/,
     4       ' TAR ',G12.5)
C
C
C  DETERMINE THE AMOUNT OF STEAM FED TO GASIFIER
      STM = SIN(L1 + NH2O)
```

```
      WRITE(NHSTRY,*) 'STEAM FED TO GASIFIER = ', STM
C
C   CALCULATE THE TOTAL AMOUNT OF WATER IN GASIFIER
      H2OTOT = H2O + STM
C
C
C  *** CARBON BALANCE ***
C
      GCARB = COMOL + CO2MOL + CH4MOL + 2.D0*(C2H4MOL+C2H6MOL) +
     &          10.D0*TARMOL + 2.D0*(C2H2MOL)
      CCARB = TCARB - GCARB
      WRITE(NHSTRY,996) TCARB,GCARB,CCARB
  996 FORMAT(/,' TOTAL CARBON= ',G12.5,/,' GASEOUS CARBON= ',G12.5,
     &       /,' CHAR CARBON= ',G12.5)
      IF ( CCARB .LE. 0.D0) THEN
        CFACT  = TCARB/GCARB
        CCARB = 0.D0
        ISEV=3
        IF (MERRPT(IPROG,IDS,ISEV,8600001,LMSG,KFLAG).NE.0)
     &  WRITE(NHSTRY,162) CFACT
  162   FORMAT(6X,'PREDICTED GASEOUS CARBON YIELD EXCEEDS CARBON
     &  AVAILABLE ',/,
     &  6X,' GASEOUS CARBON COMPOUND YIELD ADJUSTED BY A FACTOR OF ',
     &  G12.5,' AND CHAR CARBON SET TO ZERO')
C       CALL ERRSP(ISEV,3)
  163   COMOL   = CFACT * COMOL
        CO2MOL  = CFACT * CO2MOL
        CH4MOL  = CFACT * CH4MOL
        C2H4MOL = CFACT * C2H4MOL
        C2H6MOL = CFACT * C2H6MOL
C       C6H6MOL = CFACT * C6H6MOL
        TARMOL  = CFACT * TARMOL
      END IF
C
C  ***  OXYGEN BALANCE ***
C
C     write(nhstry,*) ' oxy1 =  ',oxy
      OAVAIL = 2.D0*SIN(L1 + NO2) + TOXY + H2OTOT
C REAL(6) IS MOL% OF O IN WOOD RETAINED IN CHAR
      COXY = TOXY * (REAL(6)/100.D0)
      OREQD = COMOL + 2.D0*CO2MOL + COXY
      WRITE(NHSTRY,993) COMOL,CO2MOL,COXY,OAVAIL,OREQD
  993 FORMAT(/,' COMOL = ',G12.5,' CO2MOL = ',G12.5,' COXY = ',G12.5,
     &       /,' OAVAIL = ',G12.5,' OREQD = ',G12.5,/)
       IF (OREQD .GT. TOXY) THEN
        STMDEC = (OREQD - TOXY)
        H2OTOT = H2OTOT - STMDEC
        IF (H2OTOT .LT. 0) THEN
          WRITE(NHSTRY,*) 'NEED MORE STEAM '
        ENDIF
        WRITE (NHSTRY,994) STMDEC
  994 FORMAT(/,' STEAM DECOMPOSITION = ',G12.5,' MOLES',/)
        OXY = 0
       ELSE IF (OREQD .LT. TOXY) THEN
```

```
C      write(nhstry,*) ' oxy2 =  ',oxy
       OXY = TOXY - OREQD
C      write(nhstry,*) ' oxy3 =  ',oxy
      ELSE
       WRITE(NHSTRY,*) 'OXYGEN BALANCE ALL MESSED UP '
      ENDIF
      IF (OXY .GT. 0) THEN
        WRITE(NHSTRY,*) 'MOLES OF ADDITIONAL OXYGEN (O) TO CHAR = ',OXY
        COXY = COXY + OXY
        OXY = 0
      ENDIF
C
C
C  *** HYDROGEN BALANCE ***
C
      AMMOL = TRNIT * (1.D0 - REAL(3)/100.D0)
      CNIT = TRNIT * (REAL(3)/100.D0)
      H2SMOL = TSULF * ( 1.D0 - REAL(4)/100.D0 )
      CSULF = TSULF * (REAL(4)/100.D0)
C
C REAL(5) IS H/C MASS RATIO IN CHAR
C
      CHRHYD = ( CCARB*CAW * REAL(5) ) / HAW

      GASHYD = 2.D0*H2MOL + 4.D0*CH4MOL + 6.D0*(C2H6MOL) +
     &       3*AMMOL + 2*H2SMOL + 8*TARMOL + 4*C2H4MOL + 2*C2H2MOL
      HREQD = GASHYD + CHRHYD
      HAVAIL = THYD + STMDEC*2.D0
      WRITE(NHSTRY,995)AMMOL,H2SMOL,GASHYD,CHRHYD,HAVAIL,HREQD
  995 FORMAT(/,' MOLES',/,' NH3 ',G12.5,' H2S ',G12.5,
     &       ' GASEOUS HYDROGEN',G12.5,/,' CHAR HYDROGEN ',G12.5,
     &       ' AVAIL. HYDROGEN',G12.5,
     &       ' REQ. HYDROGEN',G12.5)
      IF (HREQD .GT. HAVAIL) THEN
       WRITE(NHSTRY,*) ' ERROR: NOT ENOUGH HYDROGEN AVAILABLE'
        ISEV=1
        IF (MERRPT(IPROG,IDS,ISEV,8600001,LMSG,KFLAG).NE.0)
     &  WRITE(NHSTRY,164)
  164   FORMAT(6X,'PREDICTED HYDROGEN YIELD EXCEEDS HYDROGEN AVAILABLE '
     &  ,/,6X,' STEAM TO WOOD RATIO SHOULD BE INCREASED ')
C       CALL ERRSP(ISEV,3)
       ELSE IF (HREQD .GT. THYD) THEN
        WRITE (NHSTRY,950) STMDEC
  950 FORMAT(/,' NOTE: H2 BALANCE NEEDED ',G12.5, ' MOLES OF STEAM',/)
      END IF
C
C
C  FILL IN OUTLET FLOWS
C
      DO 250 I=1,NSUBS
      GOTO (200,210,220), ITYPE(I)
C
C  MIXED SUBSTREAM
C
```

```
 200 CONTINUE
     SOUT(L1 + NO2)    = OXY/2.D0
C      write(nhstry,*) ' oxy/2.0 =  ',sout(l1 + no2)
     SOUT(L1 + NCO)    = SOUT(L1 + NCO) + COMOL
     WRITE(NHSTRY,*) 'COMOLS OUT = ',SOUT(L1+NCO)
     SOUT(L1 + NCO2)   = SOUT(L1 + NCO2) + CO2MOL
     SOUT(L1 + NH2)    = SOUT(L1 + NH2) + H2MOL + STMDEC
C      SOUT(L1 + NN2)    = SOUT(L1 + NN2) + RN2
     SOUT(L1 + NH2O)   = H2OTOT
     SOUT(L1 + NH2S)   = SOUT(L1 + NH2S) + H2SMOL
     SOUT(L1 + NNH3)   = SOUT(L1 + NNH3) + AMMOL
     SOUT(L1 + NTAR)   = SOUT(L1 + NTAR) + TARMOL
     SOUT(L1 + NC2H2)  = SOUT(L1 + NC2H2) + C2H2MOL
     SOUT(L1 + NC2H6)  = SOUT(L1 + NC2H6) + C2H6MOL
     SOUT(L1 + NC2H4)  = SOUT(L1 + NC2H4) + C2H4MOL
C      SOUT(L1 + NC6H6)  = SOUT(L1 + NC6H6) + C6H6MOL
     SOUT(L1 + NCH4)  = SOUT(L1 + NCH4) + CH4MOL
C
C  FILL IN TOTAL FLOW AND AVERAGE MOLECULAR WEIGHT
C
     CALL CPACK(SOUT(IDXSUB(1)),NCP,IDX,X,FLOW)
     SOUT(L1+NCC+1)=FLOW
     SOUT(L1+NCC+9)=AVEMW(NCP,IDX,X)
     GOTO 250
C
C  CISOLID SUBSTREAM
C
 210 CONTINUE
      DO J=1 ,NCC
        SOUT(L2 + J) = SIN(L2 + J)
      ENDDO
     CALL CPACK(SOUT(IDXSUB(2)),NCP,IDX,X,FLOW)
     SOUT(L2+NCC+1)=FLOW
     SOUT(L2+NCC+9)=AVEMW(NCP,IDX,X)
     GOTO 250
C
C  NC SUBSTREAM
C
 220 CONTINUE
C
C CALCULATE CHAR FLOW AND ULTIMATE ANALYSIS
C
     CHAR = TASH+CCARB*CAW+CHRHYD*HAW+COXY*OAW+CNIT*RNAW+CSULF*SAW
     SOUT(IULTCH+1) = TASH / CHAR * 100.D0
     WRITE(NHSTRY,*) 'CHAR ASH = ',SOUT(IULTCH+1)
     SOUT(IULTCH+2) = CCARB*CAW / CHAR * 100.D0
     WRITE(NHSTRY,*) 'CHAR CARBON = ',SOUT(IULTCH+2)
     SOUT(IULTCH+3) = CHRHYD*HAW  / CHAR * 100.D0
     WRITE(NHSTRY,*) 'CHAR HYDROGEN = ',SOUT(IULTCH+3)
     SOUT(IULTCH+4) = CNIT*RNAW / CHAR * 100.D0
     WRITE(NHSTRY,*) 'CHAR NITROGEN = ',SOUT(IULTCH+4)
     SOUT(IULTCH+6) = CSULF*SAW / CHAR * 100.D0
     WRITE(NHSTRY,*) 'CHAR SULFUR = ',SOUT(IULTCH+6)
     SOUT(IULTCH+7) = COXY*OAW  / CHAR * 100.D0
```

```
      WRITE(NHSTRY,*) 'CHAR OXYGEN = ',SOUT(IULTCH+7)
C
      SOUT(L3 + NWOOD) = 1.D-10
      SOUT(L3 + NASH)  = 1.D-10
      SOUT(L3 + NCHAR) = SOUT(L3 + NCHAR) + CHAR
      TOTNC = 0.D0
      DO 230 J=1,NNCC
        TOTNC = TOTNC + SOUT(L3+J)
  230 CONTINUE
      SOUT(L3+NNCC+1) = TOTNC
  250 CONTINUE
C
C
C  ADD UP INLET ENTHALPY
C
      CALL TOTENT(SIN,NSUBS,IDXSUB,ITYPE,ENTHIN)
C
C  FIND OUTLET STREAM ENTHALPY (TP FLASH)
C
C       GUESS=1.0
C       if (SOUT(1) .lt. 0.d0) SOUT(1) = 0.d0
C       WRITE(NHSTRY,*) ' SOUT(O2)= ',SOUT(L1+NO2)
C       WRITE(NHSTRY,*) 'SOUT AND POUT WRITES'
C       DO J=1,NCC
C         WRITE(NHSTRY,*) SOUT(J)
C       ENDDO
C       WRITE(NHSTRY,*) POUT
      CALL FLASH(SOUT,NSUBS,IDXSUB,ITYPE,NBOPST,2,2,1,30,1.D-4,
     &     TOUT,POUT,GUESS,LMSG,LPMSG,IRESTR,2,RETN,IRETN,LCFLAG)
      CALL TOTENT(SOUT,NSUBS,IDXSUB,ITYPE,ENTOUT)
C
C  CALCULATE DUTY AND RETURN
C
      Q = ENTHIN-ENTOUT
      IF (LMSG.GE.4) WRITE(NHSTRY,300) ENTHIN,ENTOUT,Q
  300 FORMAT(6X,'HIN =',E13.5,'   HOUT =',E13.5,'   Q =',E13.5)
      RETURN
C
C  TERMINAL ERROR SECTION ------------------------------------
C
  820 ISEV=0
      IF (MERRPT(IPROG,IDS,ISEV,8600000,LMSG,KFLAG).EQ.0) GOTO 840
      WRITE(NHSTRY,825)
  825 FORMAT(6X,'IMPROPER STREAM STRUCTURE.'/,6X,'STREAM STRUCTURE ',
     1  'MUST BE MIXED + CISOLID + NC, IN THAT ORDER.')
C 830 CALL ERRSP(ISEV,3)
  840 RETURN
      END
```