8. Application Programs

8.1 Single Shot Programs

I-PROPATH offers the following five single shot programs.
(1) IPROPAIR calculates properties of air as a mixture of ideal gases.
(2) IPROPCHO calculates properties of complete combustion-by-air products of $C_XH_YO_Z$.
(3) IPROPIDG calculates properties of ideal gases.
(4) IPROPJNF calculates properties by JANAF-style table.
(5) IPROPKCK calculates properties by Keenan-Chao-Kaye-style gas table.

8.2 Sample Output of IPROPIDG

```
Do you need ERROR MESSAGES ? NO->0 : YES->1 = 1
This program can calculate properties of the following 54 ideal gases.

ISUB : Name of substance          | ISUB : Name of substance
   1 : NITROGEN N2                |    2 : WATER H2O
   3 : HYDROGEN H2                |    4 : NITRIC MONOXIDE NO
   5 : NITROGEN DIOXIDE NO2       |    6 : DINITROGEN MONOXIDE N2O
   7 : OXYGEN O2                  |    8 : CARBON MONOXIDE CO
   9 : CARBON DIOXIDE CO2         |   10 : METHANE CH4
  11 : PROPANE C3H8               |   12 : ETHYLENE C2H4
  13 : CHLORINE CL2               |   14 : AMMONIA H3N (NH3)
  15 : SULFUR DIOXIDE O2S (SO2)   |   16 : NEON NE
  17 : OZONE O3                   |   18 : CARBON C
  19 : HYDROGEN CHLORIDE HCL      |   20 : FLUORINE F2
  21 : HYDROGEN IODIDE HI         |   22 : HELIUM-4 HE
  23 : ARGON AR                   |   24 : HCFC22 CHCLF2
  25 : CFC13 CCLF3                |   26 : CHLOROFORM CHCL3
  27 : HCFC21 CHCL2F              |   28 : CFC12 CCL2F2
  29 : METHYLENE CLORIDE CH2CL2   |   30 : CARBON TETRAFLUORIDE CF4
  31 : METHANOL CH3-OH            |   32 : HCFC142B CH3-CCLF2
  33 : ETHYL CHLORIDE C2H5CL      |   34 : CFC114 CCLF2-CCLF2
  35 : HFC152A CH3-CHF2           |   36 : ACETYLENE C2H2
  37 : ETHANE C2H6                |   38 : n-BUTANE C4H10
  39 : ISOBUTANE C4H10            |   40 : ISOPENTANE C5H12
  98 : other substances
 Select one of ISUBs (1-40) or (98) = 98
ISUB : Name of substance          | ISUB : Name of substance
  41 : METHYL CHLORIDE CH3CL      |   42 : ACETALDEHYDE C2H4O
  43 : ACETIC ACID C2H4O2         |   44 : ETHANOL C2H6O
  45 : PROPYLENE C3H6             |   46 : ACETONE C3H6O
  47 : n-PENTANE C5H12            |   48 : BENZENE C6H6
  49 : n-HEXANE C6H14             |   50 : TOLUENE C7H8
  51 : n-HEPTANE C7H16            |   52 : n-OCTANE C8H18
  53 : ISO-OCTANE C8H18           |   54 : NAPHTHALENE C10H8
  98 : other substances           |   99 : Stop.
 Select one of ISUBs (41-54) or (98-99) = 50
 Name of Substance : TOLUENE C7H8

  KPA  PRESSURE  TEMPERATURE
   0      Pa         K
   1      bar        C
   2      bar        K
   3      Pa         C
 others   Pa         K
-----------------------------
 Select one set of units for pressure and temperature : KPA = 0
 KMOL    Amount of Substance
   0         kmol
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```
     1         kg
   others      kmol
  ------------------------------
  Select kmol or kg for amount of substance : KMOL = 0
  You can select one from the following 8 patterns of calculation
  1 : (P,T) >>> V, CP, H, S, etc |   2 : (P,V) >>> T, CP, H, S, etc
  3 : (T,V) >>> P, CP, H, S, etc |   4 : (P,S) >>> T, V, CP, H, etc
  5 : (T,S) >>> P, V, CP, H, etc |   6 : (V,S) >>> P, T, CP, H, etc
  7 : (P,H) >>> T, V, CP, S, etc |   8 : (P,U) >>> T, V, CP, S, etc
  Input INDEX for pattern of calculation (1-8) = 1
  Name of Substance : TOLUENE C7H8

  INPUT P[Pa]  = 1.0E+06
  INPUT T[K] = 500
   AMM=    92.14100[kg/kmol]    T  =     500.000[K]
   P  = 0.10000E+07[Pa]         V  = 0.41573E+01[m^3/kmol]
   CP = 0.17078E+06[J/(kmol*K)] CV = 0.16246E+06[J/(kmol*K)]
   W  = 0.21778E+03[m/s]        S  = 0.37141E+06[J/(kmol*K)]
   H  = 0.28222E+08[J/kmol]     U  = 0.24065E+08[J/kmol]
   ------------------------------------------------------
   1 : CONTINUE                 2 : SELECT PATTERN OF CALCULATION
   3 : SELECT SYSTEM OF UNITS   4 : SELECT SUBSTANCE
   5 : STOP
  What do you wish to do next ? Input (1-5) = 2
  You can select one from the following 8 patterns of calculation
  1 : (P,T) >>> V, CP, H, S, etc |   2 : (P,V) >>> T, CP, H, S, etc
  3 : (T,V) >>> P, CP, H, S, etc |   4 : (P,S) >>> T, V, CP, H, etc
  5 : (T,S) >>> P, V, CP, H, etc |   6 : (V,S) >>> P, T, CP, H, etc
  7 : (P,H) >>> T, V, CP, S, etc |   8 : (P,U) >>> T, V, CP, S, etc
  Input INDEX for pattern of calculation (1-8) = 6
  Name of Substance : TOLUENE C7H8

  INPUT V[m^3/kmol] = 4.1573
  INPUT S[J/(kmol*K)] = 0.37141E+06
   AMM=    92.14100[kg/kmol]    T  =     500.009[K]
   P  = 0.10000E+07[Pa]         V  = 0.41573E+01[m^3/kmol]
   CP = 0.17078E+06[J/(kmol*K)] CV = 0.16246E+06[J/(kmol*K)]
   W  = 0.21778E+03[m/s]        S  = 0.37141E+06[J/(kmol*K)]
   H  = 0.28223E+08[J/kmol]     U  = 0.24066E+08[J/kmol]
   ------------------------------------------------------
   1 : CONTINUE                 2 : SELECT PATTERN OF CALCULATION
   3 : SELECT SYSTEM OF UNITS   4 : SELECT SUBSTANCE
   5 : STOP
  What do you wish to do next ? Input (1-5) = 5
Stop - Program terminated.
```

8.3 Example of User's PROGRAM UNIT (IPROPJNF.FOR)

Source program

```
C *****
C  This propram calculates properties of ideal gases
C  in order to produce a JANAF style gas table
      CHARACTER*25 ANAME,IDENTI
      INTEGER IERR,ISUB
      REAL T
      REAL C(1:10)
      REAL A(1:4)
      COMMON /UNIT/KPA,KGM,MESS
      COMMON /CNST/GASCON
      CHARACTER*25 AANAME(54)
      INTEGER IP(54)
      ISUBNO=54
      IDISP=40
```

```
      WRITE(6,2200)
 2200 FORMAT(1H ,' Do you need ERROR MESSAGES ? NO->0 : YES->1 = ')
      READ(5,*) IM
      CALL IPINIT(0,0,IM,0,0.0)
      DO 10 I=1,ISUBNO
      IP(I)=I
      AANAME(I)=IDENTI(I,'S')
   10 CONTINUE
  100 WRITE(6,2100) ISUBNO
 2100 FORMAT(1H ,' This program can calculate properties of ',
     1 'the following ',I2,' ideal gases.'//
     2 1h ,1X,'ISUB : Name of substance',10X,
     3      '| ISUB : Name of substance')
      DO 20 I=1,IDISP,2
      WRITE(6,2110) IP(I),AANAME(I),IP(I+1),AANAME(I+1)
 2110 FORMAT(1H ,2X,I3,' : ',A25,'  |  ',I3,' : ',A25)
   20 CONTINUE
      WRITE(6,2120) IDISP
 2120 FORMAT(1H ,3X,'98 : other substances'
     1/3X,'Select one of ISUBs (1-',I2,') or (98) = ')
      READ(5,*) ISUB
      IF (ISUB .LT. 1 .OR. ISUB .GT. IDISP) THEN
      WRITE(6,2140)
 2140 FORMAT(2X,'ISUB : Name of substance',10X,
     1      '| ISUB : Name of substance')
      DO 30 I=IDISP+1,ISUBNO,2
      WRITE(6,2110) IP(I),AANAME(I),IP(I+1),AANAME(I+1)
   30 CONTINUE
      WRITE(6,2160) IDISP+1,ISUBNO
 2160 FORMAT(1H ,3X,'98 : other substances',11X,
     1 '|   99 : Stop.'/
     2 3X,'Select one of ISUBs (',I2,'-',I2,') or (98-99) = ')
      READ(5,*) ISUB
      ENDIF
      ANAME=IDENTI(ISUB,'S')
      IF (ISUB .LT. 1 .OR. ISUB .GT. ISUBNO) THEN
        IF (ISUB .EQ. 98) THEN
          GOTO 100
        ELSE
          STOP
        ENDIF
      ENDIF
      WRITE(6,2000) ANAME
 2000 FORMAT(1H , ' Name of Substance : ',A25)
      CALL IDGFND(IERR,ISUB,C,ANAME)
      AMM=C(1)
      WRITE(6,2300) AMM,C(2),C(3),C(4)
      AKF=-C(7)/(298.15*GASCON)/ALOG(10.0)
      WRITE(6,2320) C(5),C(6),C(7),ANAME,AKF
 2300 FORMAT(3X,'  Molecular weight     = ', F13.4/
     1 3X,'  Critical temperature = ',F13.3, '[K]'/
     2 3X,'  Critical pressure    = ',E13.5, '[Pa]'/
     3 3X,'  Critical volume      = ',E13.5, '[m**3/kmol]')
 2320 FORMAT(1H ,' At reference state of 0.1MPa and 298.15 K'/
     1 3X,'  Absolute entropy          = ',E13.5,'[J/(kmol*K)]'/
     1 3X,'  Enthalpy of formation     = ',E13.5,'[J/kmol]'/
     1 3X,'  Gibbs energy of formation = ',E13.5,'[J/kmol]'/
     1 3X,'  Logarithm of the equilibrium constant of the reaction '/
     1 3X,'  for the formation of ',A25/
     1 3X,'  from the elements:log(Kf) = ',F10.4/)
  200 WRITE(6,*) ' INPUT T [K] = '
      READ(5,*) T
      CALL IDGT(IERR,ISUB,T,A,ANAME)
      CP=A(1)
      CV=CP-GASCON
      WSOUND=SQRT(CP/CV*GASCON/AMM*T)
      S=A(2)
      GREF=A(3)
      H=A(4)
      U=H-GASCON*T
```

```
     WRITE(6,1000) ANAME,T,CP,S,GREF,H,CV,WSOUND
1000 FORMAT(1H ,' Substance : ',A25/
    1 3X,'                    T  = ',F12.3,'[K]'/
    2 3X,'                CP(T) = ',E12.6,'[J/(kmol*K)]'/
    2 3X,'                S0(T) = ',E12.6,'[J/(kmol*K)]'/
    3 3X,'-(G0(T)-H0(298.15K))/T = ',E12.6,'[J/(kmol*K)]'/
    4 3X,'      H(T)-H(298.15K)  = ',E12.6,'[J/kmol]'/
    5 3X,'                CV(T) = ',E12.6,'[J/(kmol*K)]'/
    6 3X,'                W     = ',E12.6,'[m/s]'/
    7 3X,'-----------------------------------------------')
     WRITE(6,*) ' 1:CONTINUE  |  2:SELECT SUBSTANCE  |  3:STOP '
     WRITE(6,*) ' What do you wish to do next ? Input (1-3) =  '
     READ(5,*) INUM
     IF (INUM .EQ. 1) THEN
       GOTO 200
     ELSEIF (INUM .EQ. 2) THEN
       GOTO 100
     ENDIF
     STOP
     END
```

Sample output

```
 Do you need ERROR MESSAGES ? NO->0 : YES->1 = 1
 This program can calculate properties of the following 54 ideal gases.

 ISUB : Name of substance          | ISUB : Name of substance
    1 : NITROGEN N2                |    2 : WATER H2O
    3 : HYDROGEN H2                |    4 : NITRIC MONOXIDE NO
    5 : NITROGEN DIOXIDE NO2       |    6 : DINITROGEN MONOXIDE N2O
    7 : OXYGEN O2                  |    8 : CARBON MONOXIDE CO
    9 : CARBON DIOXIDE CO2         |   10 : METHANE CH4
   11 : PROPANE C3H8               |   12 : ETHYLENE C2H4
   13 : CHLORINE CL2               |   14 : AMMONIA H3N (NH3)
   15 : SULFUR DIOXIDE O2S (SO2)   |   16 : NEON NE
   17 : OZONE O3                   |   18 : CARBON C
   19 : HYDROGEN CHLORIDE HCL      |   20 : FLUORINE F2
   21 : HYDROGEN IODIDE HI         |   22 : HELIUM-4 HE
   23 : ARGON AR                   |   24 : HCFC22 CHCLF2
   25 : CFC13 CCLF3                |   26 : CHLOROFORM CHCL3
   27 : HCFC21 CHCL2F              |   28 : CFC12 CCL2F2
   29 : METHYLENE CLORIDE CH2CL2   |   30 : CARBON TETRAFLUORIDE CF4
   31 : METHANOL CH3-OH            |   32 : HCFC142B CH3-CCLF2
   33 : ETHYL CHLORIDE C2H5CL      |   34 : CFC114 CCLF2-CCLF2
   35 : HFC152A CH3-CHF2           |   36 : ACETYLENE C2H2
   37 : ETHANE C2H6                |   38 : n-BUTANE C4H10
   39 : ISOBUTANE C4H10            |   40 : ISOPENTANE C5H12
   98 : other substances
  Select one of ISUBs (1-40) or (98) = 2
 Name of Substance : WATER H2O
    Molecular weight     =       18.0150
    Critical temperature =       647.130[K]
    Critical pressure    =   0.22055E+08[Pa]
    Critical volume      =   0.55950E-01[m**3/kmol]
 At reference state of 0.1MPa and 298.15 K
    Absolute entropy          =   0.18872E+06[J/(kmol*K)]
    Enthalpy of formation     =  -0.24181E+09[J/kmol]
    Gibbs energy of formation =  -0.22859E+09[J/kmol]
    Logarithm of the equilibrium constant of the reaction
    for the formation of WATER H2O
    from the elements:log(Kf) =    40.0470

 INPUT T [K] = 300
 Substance : WATER H2O
                      T  =      300.000[K]
                  CP(T) = 0.335859E+05[J/(kmol*K)]
                  S0(T) = 0.188928E+06[J/(kmol*K)]
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```
 -(G0(T)-H0(298.15K))/T = 0.188721E+06[J/(kmol*K)]
       H(T)-H(298.15K)  = 0.621280E+05[J/kmol]
                  CV(T) = 0.252714E+05[J/(kmol*K)]
                  W     = 0.428969E+03[m/s]
 ------------------------------------------------
1:CONTINUE  |  2:SELECT SUBSTANCE  |  3:STOP
What do you wish to do next ? Input (1-3) =  1
INPUT T [K] = 500
Substance : WATER H2O
                     T  =      500.000[K]
                  CP(T) = 0.352270E+05[J/(kmol*K)]
                  S0(T) = 0.206414E+06[J/(kmol*K)]
 -(G0(T)-H0(298.15K))/T = 0.192569E+06[J/(kmol*K)]
       H(T)-H(298.15K)  = 0.692221E+07[J/kmol]
                  CV(T) = 0.269125E+05[J/(kmol*K)]
                  W     = 0.549600E+03[m/s]
 ------------------------------------------------
1:CONTINUE  |  2:SELECT SUBSTANCE  |  3:STOP
What do you wish to do next ? Input (1-3) =  2
This program can calculate properties of the following 54 ideal gases.

ISUB : Name of substance          | ISUB : Name of substance
   1 : NITROGEN N2                |    2 : WATER H2O
   3 : HYDROGEN H2                |    4 : NITRIC MONOXIDE NO
   5 : NITROGEN DIOXIDE NO2       |    6 : DINITROGEN MONOXIDE N2O
   7 : OXYGEN O2                  |    8 : CARBON MONOXIDE CO
   9 : CARBON DIOXIDE CO2         |   10 : METHANE CH4
  11 : PROPANE C3H8               |   12 : ETHYLENE C2H4
  13 : CHLORINE CL2               |   14 : AMMONIA H3N (NH3)
  15 : SULFUR DIOXIDE O2S (SO2)   |   16 : NEON NE
  17 : OZONE O3                   |   18 : CARBON C
  19 : HYDROGEN CHLORIDE HCL      |   20 : FLUORINE F2
  21 : HYDROGEN IODIDE HI         |   22 : HELIUM-4 HE
  23 : ARGON AR                   |   24 : HCFC22 CHCLF2
  25 : CFC13 CCLF3                |   26 : CHLOROFORM CHCL3
  27 : HCFC21 CHCL2F              |   28 : CFC12 CCL2F2
  29 : METHYLENE CLORIDE CH2CL2   |   30 : CARBON TETRAFLUORIDE CF4
  31 : METHANOL CH3-OH            |   32 : HCFC142B CH3-CCLF2
  33 : ETHYL CHLORIDE C2H5CL      |   34 : CFC114 CCLF2-CCLF2
  35 : HFC152A CH3-CHF2           |   36 : ACETYLENE C2H2
  37 : ETHANE C2H6                |   38 : n-BUTANE C4H10
  39 : ISOBUTANE C4H10            |   40 : ISOPENTANE C5H12
  98 : other substances
 Select one of ISUBs (1-40) or (98) = 98
ISUB : Name of substance          | ISUB : Name of substance
  41 : METHYL CHLORIDE CH3CL      |   42 : ACETALDEHYDE C2H4O
  43 : ACETIC ACID C2H4O2         |   44 : ETHANOL C2H6O
  45 : PROPYLENE C3H6             |   46 : ACETONE C3H6O
  47 : n-PENTANE C5H12            |   48 : BENZENE C6H6
  49 : n-HEXANE C6H14             |   50 : TOLUENE C7H8
  51 : n-HEPTANE C7H16            |   52 : n-OCTANE C8H18
  53 : ISO-OCTANE C8H18           |   54 : NAPHTHALENE C10H8
  98 : other substances           |   99 : Stop.
 Select one of ISUBs (41-54) or (98-99) = 52
Name of Substance : n-OCTANE C8H18
   Molecular weight     =      114.2310
   Critical temperature =       568.700[K]
   Critical pressure    =   0.24900E+07[Pa]
   Critical volume      =   0.48600E+00[m**3/kmol]
At reference state of 0.1MPa and 298.15 K
   Absolute entropy          =   0.46723E+06[J/(kmol*K)]
   Enthalpy of formation     =  -0.20875E+09[J/kmol]
   Gibbs energy of formation =   0.16000E+08[J/kmol]
   Logarithm of the equilibrium constant of the reaction
   for the formation of n-OCTANE C8H18
   from the elements:log(Kf) =    -2.8031

INPUT T [K] = 500
Substance : n-OCTANE C8H18
                     T  =      500.000[K]
                  CP(T) = 0.287545E+06[J/(kmol*K)]
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```
                  S0(T) = 0.588724E+06[J/(kmol*K)]
  -(G0(T)-H0(298.15K))/T = 0.492094E+06[J/(kmol*K)]
       H(T)-H(298.15K)  = 0.483151E+08[J/kmol]
                  CV(T) = 0.279231E+06[J/(kmol*K)]
                  W     = 0.193590E+03[m/s]
  ------------------------------------------------
 1:CONTINUE  |  2:SELECT SUBSTANCE  |  3:STOP
 What do you wish to do next ? Input (1-3) =  3
Stop - Program terminated.
```

References

[1] Daubert, T. E. and Danner, R.P., Physical and Thermodynamic Properties of Pure Chemicals, data compilation, Design Institute for Physical Property Data Americal Institute of Chemical Engineers, Hemisphere, (1991).

[2] Keenan, J. P., Chao, J. and Kaye, J, Gas Tables, 2nd. ed. (SI Units), Wiley, (1983).

[3] Chase, Jr.,M.W. et al., JANAF Thermochemical Tables, 3rd ed., J. Physical and Chemical Reference Data, Vol.14(1985), supplement No.1.