2.2 Ammonia–Water(Tillner-Roth and Friend)

Thermodynamic properties are evaluated by the formulation of Tillner-Roth et al. [1]. This uses the water equation of state by Pruss et al. [2] and ammonia equation of state by Tillner-Roth et al. [3]. No provision is made for transport properties at this moment.

Notice

This program has some problems in high pressure region. The calculation in the region may not terminate successfully from time to time.

2.2.1 Temperature Scale

International temperature scale 1990 (ITS-1990)

2.2.2 The Names of Substance, Library File and Single Shot Program

Substance:	Ammonia-Water Mixture
First Component:	Ammonia
Second Component:	Water
Library File for UNIX:	`libjawmx2.a`
Library File for DOS,Windows95/NT:	JAWMX2.LIB
Single Shot Program for UNIX:	`awmx2-ss`
Single Shot Program for DOS,Windows95/NT:	AWMX2–SS.EXE

2.2.3 Important Constants and Others

Table IV-2.2-1 Molecular Formula,Relative Molecular Mass and Gas Constant

	Molecular Formula	Relative Molecular Mass	Gas Constant
Ammonia	NH_3	17.03026kg/kmol	488.189×10^3J/(kg·K)
Water	H_2O	18.015268kg/kmol	461.5189×10^3J/(kg·K)

Table IV-2.2-2 Critical Constant

	Critical temperature	Critical pressure	Critical specific volume
Ammonia	405.40K 132.25°C	11.36×10^6Pa 113.6bar	75.7×10^{-3}m^3/kmol 4.44×10^{-3}m^3/kg
Water	647.096K 373.946°C	22.064×10^6Pa 220.64bar	55.9×10^{-3}m^3/kmol 3.11×10^{-3}m^3/kg

Table IV-2.2-3 Reference State Specified by `KSTAN`

KSTAN	Values of enthalpy (or internal energy) and entropy at the reference state
0	Comforms to reference[1] For saturated liquid at the triple-point temperature of both pure components , 273.16 K for water and 195.495 K for ammonia , the internal energy and entropy have been set as : u=0 and s=0
1	Enthalpy and entropy of saturated liquid of pure ammonia at 273.15K 200kJ/kg and 1kJ/(kg·K), respectively Enthalpy and entropy of saturated liquid of pure water at 273.15K 200kJ/kg and 1kJ/(kg·K), respectively
others	The same with when KSTAN=0

2.2.4 Formula

No correction has been made to the original formulations.

2.2.5 Valid Range

$$0.01[\text{bar}]<p<400[\text{bar}]$$
$$200[\text{K}]<T<620[\text{K}]$$

2.2.6 Example of User's PROGRAM UNIT

Sample Program 1

example1.for :

```
c       ------------------------------------------------
c         This program calculateds temperature at bubble
c         points (p=10[bar])from z=0.0 to 1.0 [kg NH3/kg]
c         at every 0.1 [kg NH3/kg] interval.
c       ------------------------------------------------

      REAL T,P,Z,H,S
      INTEGER I,J

      CALL KPAMES(1,1)
      CALL STNKAS(1,1)

c      ------------------------------------------------
c         bubble point pressure using
c         subtb.
C      ------------------------------------------------
      P=10.0
      DO 10 I=0,10
              Z=FLOAT(I)*0.1
              CALL SUBTB(J,T,P,Z,V,H,S)
              WRITE(*,*) Z,T
10    CONTINUE
      STOP
      END

C
c -----------------------------------------
c Results
c -----------------------------------------
c 0.000000E+00 179.877300
c 1.000000E-01 149.922400
c 2.000000E-01 125.212800
c 3.000000E-01 101.825800
c 4.000000E-01  80.509940
c 5.000000E-01  62.563330
c 6.000000E-01  48.753480
c 7.000000E-01  39.080770
c 8.000000E-01  32.721220
c 9.000000E-01  28.394670
c     1.000000  24.894940
```

Sample Program 2

example2.for :

```
c    -------------------------------------------
c      This program calculates the properties in
c      saturated state at 5.0[bar], T=300[K]
c    -------------------------------------------
```

```
      REAL T,P,X,Y,VL,VV,HL,HV,SL,SV
      INTEGER J

c     ------------------------------------------
c          T=[K], P=[Pa]
c          standard state=(bibliography [1])
c          unit of quantity=[kmol]
c     ------------------------------------------

      CALL KPAMES(0,1)
      CALL STNKAS(0,0)

c     ------------------------------------------
c        Properties in saturated state
c     ------------------------------------------
      P=5.0E5
      T=300.0
      CALL SUBXY(J,T,P,X,Y,VL,VV,HL,HV,SL,SV)
      IF(J.NE.0) THEN
             WRITE(*,*) 'ERROR IN SUBXY J=',J
      ELSE
             HL=HL*1.0E-6
             HV=HV*1.0E-6
             SL=SL*1.0E-3
             SV=SV*1.0E-3
             WRITE(*,*) ' X[kmol NH3/kmol]=',X, '  Y[kmol NH3/kmol]=',Y
             WRITE(*,*) 'VL[M^3/kmol]     =',VL,' VV[M^3/kmol]     =',VV
             WRITE(*,*) 'HL[MJ/kmol]      =',HL,' HV[MJ/kmol]      =',HV
             WRITE(*,*) 'SL[MJ/(kmol.K)]  =',SL,' SV[MJ/(kmol.K)]  =',SV
      ENDIF
      STOP
      END
C
c     ---------------------------------------------------------------
c Results
c     ---------------------------------------------------------------
c     X[kmol NH3/kmol]=   6.012722E-01  Y[kmol NH3/kmol]=   9.987947E-01
c    VL[M^3/kmol]     =   2.212924E-02 VV[M^3/kmol]     =       4.723189
c    HL[MJ/kmol]      =       1.458077 HV[MJ/kmol]      =      28.437260
c    SL[MJ/(kmol.K)]  =      18.430890 SV[MJ/(kmol.K)]  =     106.415300
```

2.2.7 Sample Output of Single Shot Program

```
=====================================================================
|   Single Shot Program for Ammonia-Water Mixture,                   |
|   an Application Program by M-PROPATH Ver.11.1                      |
|   Thermophysical Properties of Ammonia-Water Mixtures               |
|---------------------------------------------------------------------|
|  ## First Menu ##                                                   |
| No.                      Current                                    |
| 1 --> Go to Second Menu                                             |
| 2 --> Read Help                                                     |
| 3 --> Set Logfile       [OFF]                                       |
| 0 --> Quit                                                          |
=====================================================================
Input No.
2

 This is help for this program (AWMX-SS2.EXE)
  Nomenclature
 ==== First Charactor ====
   H : Enthalpy
   P : Pressure
```

```
   S : Entropy
   T : Temperature
   V : Volume
   X : Ammonia Composition of Liquid
   Y : Ammonia Composition of Vapor
   Z : Total Composition of Ammonia
 ==== Second Charactor ====
   B : Bubble Point
   D : Dew Point
   L : Liquid
   V : Vapor

----- Hit RETURN Key -----

=========================================================================
|   Single Shot Program for Ammonia-Water Mixture,                      |
|   an Application Program by M-PROPATH Ver.11.1                        |
|   Thermophysical Properties of Ammonia-Water Mixtures                 |
|-----------------------------------------------------------------------|
|  ## First Menu ##                                                     |
| No.                    Current                                        |
| 1 --> Go to Second Menu                                               |
| 2 --> Read Help                                                       |
| 3 --> Set Logfile       [OFF]                                         |
| 0 --> Quit                                                            |
=========================================================================
Input No.
3

 1: Logfile ON
 2: Logfile OFF
Input No.
1
Input Filename
AWMIX.LOG
=========================================================================
|   Single Shot Program for Ammonia-Water Mixture,                      |
|   an Application Program by M-PROPATH Ver.11.1                        |
|   Thermophysical Properties of Ammonia-Water Mixtures                 |
|-----------------------------------------------------------------------|
|  ## First Menu ##                                                     |
| No.                    Current                                        |
| 1 --> Go to Second Menu                                               |
| 2 --> Read Help                                                       |
| 3 --> Set Logfile       [ON] SAMPLE.LOG                               |
| 0 --> Quit                                                            |
=========================================================================
Input No.
1
============================================================
| ## Second Menu ##                                        |
|  <Single and Two Phase States>                           |
| No.  Input                  Output                       |
| 1 --(P,T,Z)-->    H  HL HV S  SL SV V  VL VV X  Y  QUALITY  |
| 2 --(P,Z,H)--> T     HL HV S  SL SV V  VL VV X  Y  QUALITY  |
| 3 --(P,Z,S)--> T  H  HL HV    SL SV V  VL VV X  Y  QUALITY  |
| 4 --(P,Z,V)--> T  H  HL HV S  SL SV    VL VV X  Y  QUALITY  |
|----------------------------------------------------------|
|  <Two Phase State>                                       |
| 5 --(P,Z)----> X=Z : TB HB SB VB    Y=Z : TD HD SD VD    |
| 6 --(T,Z)----> X=Z : PB HB SB VB    Y=Z : PD HD SD VD    |
| 7 --(P,T)----> Coexisting Phases: X  Y  HL HV SL SV VL VV |
|----------------------------------------------------------|
| 8 -----------> Fundamental Constants                     |
| 9 -----------> Conversion of Composition and Relative    |
|                Molcular Mass of Mixture                  |
|10 -----------> Change System of Unit, and Standard Values of|
|                Enthalpy and Entropy                      |
|99 -----------> Return to First Menu                      |
| 0 -----------> Quit                                      |
============================================================
```

```
Input No.
10

=====================================================
 No.                                 current
=====================================================
 1 --> Pressure and Temperature    [bar, C]
 2 --> Amount of Substance         [kmol]
 3 --> Standard Values of h and s  [2]
 0 --> Return to Second Menu
=====================================================
Input No.
1

==============================
 No.  <Pressure> <Temperature>
==============================
 1 -->   Pa            K
 2 -->   bar           C
 3 -->   bar           K
 4 -->   Pa            C
==============================
Input No.
2

=====================================================
 No.                                 current
=====================================================
 1 --> Pressure and Temperature    [ bar, C]
 2 --> Amount of Substance         [kmol]
 3 --> Standard Values of h and s  [2]
 0 --> Return to Second Menu
=====================================================
Input No.
2

===========================
 No.   Amount of Substance
 1 -->   kmol
 2 -->   kg
===========================
Input No.
2

=====================================================
 No.                                 current
=====================================================
 1 --> Pressure and Temperature    [ bar, C]
 2 --> Amount of Substance         [ kg ]
 3 --> Standard Values of h and s  [2]
 0 --> Return to Second Menu
=====================================================
Input No.
3

=============================================
 No.   Standard States and Values of h and s
 1 --> As defined in :
       Reiner Tillner-Roth and Daniel G. Friend
       A Helmholtz  Free Energy Formulation  of
       the  Thermodynamic Properties  of  the
       Mixtures {Water + Ammonia}, Journal of
       Physical and Chemical Reference Data,
       27-1,(1996),pp63-96
 2 --> Convention of International Institute of
       Refrigeration(IIR):
       h=200[kJ/kg], s=1.0[kJ/(kg*K)]
       Saturated Pure Liquids at 0[C]
=============================================
Input No.
1
```

```
=====================================================
 No.                                current
=====================================================
 1 --> Pressure and Temperature    [ bar, C]
 2 --> Amount of Substance         [ kg ]
 3 --> Standard Values of h and s  [1] T-Roth & Friend
 0 --> Return to Second Menu
=====================================================
Input No.
0
============================================================
| ## Second Menu ##                                        |
 contents not shown
============================================================
Input No.
9

================================================================
 Conversion of Composition and Relative Molecular Mass of Mixture
================================================================

 1: [kmol/kmol] --> [kg/kg]     and Relative Molecular Mass of Mixture
 2: [kg/kg]     --> [kmol/kmol] and Relative Molecular Mass of Mixture
 0: Return to Second Menu
Input No.
1
Input Z[kmol/kmol]
0.5
 Z  =    .50000000[kmol/kmol]
 Z  =    .48594670[kg/kg]
 Relative Molecular Mass of Mixture =      17.52276000[kg/kmol]
 Relative Molecular Mass of Ammonia =      17.03026000[kg/kmol]
 Relative Molecular Mass of Water   =      18.01527000[kg/kmol]


 1: [kmol/kmol] --> [kg/kg]     and Relative Molecular Mass of Mixture
 2: [kg/kg]     --> [kmol/kmol] and Relative Molecular Mass of Mixture
 0: Return to Second Menu
Input No.
2
Input Z[kg/kg]
0.5
 Z  =    .50000000[kg/kg]
 Z  =    .51405330[kmol/kmol]
 Relative Molecular Mass of Mixture =      17.50892000[kg/kmol]
 Relative Molecular Mass of Ammonia =      17.03026000[kg/kmol]
 Relative Molecular Mass of Water   =      18.01527000[kg/kmol]


 1: [kmol/kmol] --> [kg/kg]     and Relative Molecular Mass of Mixture
 2: [kg/kg]     --> [kmol/kmol] and Relative Molecular Mass of Mixture
 0: Return to Second Menu
Input No.
0
============================================================
| ## Second Menu ##                                        |
 contents not shown
============================================================
Input No.
8

======================
 Fundamental Constants
======================
    <Constants>               <Ammonia>       <Water>
Relative Molecular Mass       17.03026000     18.01527000  [kg/kmol]
Gas Constants                488.18900000    461.51890000  [J/(kg*K)]
Critical Temperature         405.40000000    647.09600000  [K]
                             132.25000000    373.94600000  [C]
Critical Pressure            113.60000000    220.64000000  [bar]
```

```
Critical Volume             .75690050E-01   .55948040E-01  [m**3/kmol]
                            .44444450E-02   .31055900E-02  [m**3/kg]
----- Hit RETURN Key -----

============================================================
| ## Second Menu ##                                        |
 contents not shown
============================================================
Input No.
1

====================================
 (P,T,Z) --> H, S, V, QUALITY
             X, HL, SL, VL
             Y, HV, SV, VV
====================================
Input P[bar]          (P=0 : Second Menu)
1
Input T[C]
200
Input Z[kg/kg]
0.5
T  =     200.00000000[C]          P  =       1.00000000[bar]
Z  =        .50000000[kg/kg]      H  =    2481.23400000[kJ/kg]
S  =       8.30849400[kJ/(kg.K)]  V  =    .22386150E+01[m**3/kg]
Vapor Region

Input P[bar]          (P=0 : Second Menu)
1
Input T[C]
50.0
Input Z[kg/kg]
0.5
 T  =      50.00000000[C]          P  =       1.00000000[bar]
 Z  =         .50000000[kg/kg]     H  =     875.56820000[kJ/kg]
 S  =       3.75734900[kJ/(kg*K)]  V  =    .68341210E+00[m**3/kg]
 X  =         .18624860[kg/kg]     Y  =        .90054950[kg/kg]
 HL =     130.32380000[kJ/kg]      HV =    1826.98200000[kJ/kg]
 SL =     912.73970000[J/(kg*K)]   SV =       7.38890700[kJ/(kg*K)]
 VL =    .10951560E-02[m**3/kg]    VV =    .15544890E+01[m**3/kg]
 QUALITY =       .43924260[kg/kg]

Input P[bar]          (P=0 : Second Menu)
0
============================================================
| ## Second Menu ##                                        |
 contents not shown
============================================================
Input No.
2

====================================
 (P,Z,H) --> T, S, V, QUALITY
             X, HL, SL, VL
             Y, HV, SV, VV
====================================
Input P[bar]          (P=0 : Second Menu)
1
Input Z[kg/kg]
0.5
Input H[kJ/kg]
2500.
 T  =     208.52500000[C]          P  =       1.00000000[bar]
 Z  =        .50000000[kg/kg]      H  =    2500.00000000[kJ/kg]
 S  =       8.34784100[kJ/(kg*K)]  V  =    .22795030E+01[m**3/kg]
 Vapor Region

Input P[bar]          (P=0 : Second Menu)
0
============================================================
| ## Second Menu ##                                        |
```

```
 contents not shown
============================================================
Input No.
3

====================================
 (P,Z,S) --> T, H, V, QUALITY
             X, HL, SL, VL
             Y, HV, SV, VV
====================================
Input P[bar]          (P=0 : Second Menu)
1
Input Z[kg/kg]
0.5
Input S[k/(kg*K)]
0.3
 T  =     -11.38488000[C]          P  =       1.00000000[bar]
 Z  =        .50000000[kg/kg]      H  =    -133.57350000[kJ/kg]
 S  =     300.00000000[J/(kg*K)]   V  =    .11689280E-02[m**3/kg]
 Liquid Region

Input P[bar]          (P=0 : Second Menu)
0
============================================================
| ## Second Menu ##                                        |
 contents not shown
============================================================
Input No.
4

====================================
 (P,Z,V) --> T, H, S, QUALITY
             X, HL, SL, VL
             Y, HV, SV, VV
====================================
Input P[bar]          (P=0 : Second Menu)
1.0
Input Z[kg/kg]
0.5
Input V[m**3/kg]
2.
 T  =     150.39830000[C]          P  =       1.00000000[bar]
 Z  =        .50000000[kg/kg]      H  =    2373.50700000[kJ/kg]
 S  =       8.06802600[kJ/(kg*K)]  V  =    .20000000E+01[m**3/kg]
Vapor Region

Input P[bar]          (P=0 : Second Menu)
0
============================================================
| ## Second Menu ##                                        |
 contents not shown
============================================================
Input No.
5

============================================
 (P,Z) --> X=Z : TB, HB, SB, VB
           Y=Z : TD, HD, SD, VD
============================================
Input P[bar]          (P=0 : Second Menu)
1.0
Input Z[kg/kg]
0.5
 P  =       5.00000000[bar]        Z  =        .50000000[kg/kg]
 TB =      38.31616000[C]          TD =     128.34460000[C]
 HB =      93.85913000[kJ/kg]      HD =    2303.77000000[kJ/kg]
 SB =       1.09321100[kJ/(kg*K)]  SD =       7.14666800[kJ/(kg*K)]
 VB =    .12341500E-02[m**3/kg]    VD =    .36748830E+00[m**3/kg]

Input P[bar]          (P=0 : Second Menu)
0
```

```
============================================================
| ## Second Menu ##                                        |
 contents not shown
============================================================
Input No.
6

=============================================
 (T,Z) --> X=Z : PB, HB, SB, VB
           Y=Z : PD, HD, SD, VD
=============================================
Input Z[kg/kg]   (Z < 0 : Second Menu)
0.5
Input T[K]
80.0
 T  =      80.00000000[C]          Z  =         .50000000[kg/kg]
 PB =      15.33406000[bar]        PD =         .92550240[bar]
 HB =     293.33660000[kJ/kg]      HD =    2224.19800000[kJ/kg]
 SB =       1.69010100[kJ/(kg*K)]  SD =       7.71905800[kJ/(kg*K)]
 VB =    .13032530E-02[m**3/kg]    VD =    .17920140E+01[m**3/kg]

Input Z[kg/kg]   (Z < 0 : Second Menu)
-1
============================================================
| ## Second Menu ##                                        |
 contents not shown
============================================================
Input No.
7

=============================================
 (P,T) --> Coexisting Phases
           X, HL, SL, VL
           Y, HV, SV, VV
=============================================
Input P[bar]          (P=0 : Second Menu)
1.0
Input T[C]
50.
 T  =      50.00000000[C]          P  =       1.00000000[bar]
 X  =        .18624860[kg/kg]      Y  =        .90054950[kg/kg]
 HL =     130.32380000[kJ/kg]      HV =    1826.98200000[kJ/kg]
 SL =     912.73970000[J/(kg*K)]   SV =       7.38890700[kJ/(kg*K)]
 VL =    .10951560E-02[m**3/kg]    VV =    .15544890E+01[m**3/kg]

Input P[bar]          (P=0 : Second Menu)
0
============================================================
| ## Second Menu ##                                        |
 contents not shown
============================================================
Input No.
0

***** See You Again ! *****
Stop - Program terminated.
```

References

[1] R. Tillner-Roth and D. G. Friend, Helmholtz free energy formulation of the thermodynamic properties of the mixture { water+ammonia } , Journal of Physical and Chemical Reference Data,27-1,(1996),pp63-96

[2] A. Pruss und W. Wagner, Eine neue Fundamental-gleichung fuer das fluide Zustandsgebiet von Wasser fuer Temperaturen von der Schmelzlinie bis zu 1273 K bei Druecken bis zu 1000MPa, Fortschr.-Ber. VDI 6,No.(320) (VDI verlag Duesseldorf)(1995)

[3] R. Tillner-Roth, Harms-Watzenberg und H. D. Bachr, Eine neue Fundamentalgleichung fuer Ammoniak,

Proc. 20th DKV-Tagung Heidelberg, Germany, volII,167(1993)