2. Individual Mixture and Formulation

2.1 Ammonia–Water(Ibrahim and Klein)

Thermodynamic properties are evaluated by the formulation of Ibrahim et al. [1]. No provision is made for transport properties at this moment.

2.1.1 Temperature Scale

International temperature scale 1990 (ITS-1990)

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

Substance:	Ammonia-Water Mixture
First Component:	Ammonia
Second Component:	Water
Library File fot UNIX:	`libjawmx.a`
Library File for DOS,Windows95/NT:	JAWMX.LIB
Single Shot Program for UNIX:	`awmx-ss`
Single Shot Program for DOS,Windows95/NT:	AWMX–SS.EXE

2.1.3 Important Constants and Others

Table IV-2.1-1 Molecular Formula,Relative Molecular Mass and Gas Constant

	Molecular Formula	Relative Molecular Mass	Gas Constant
Ammonia	NH_3	17.03026kg/kmol	488.2197×10^3J/(kg·K)
Water	H_2O	18.0153kg/kmol	461.5249×10^3J/(kg·K)

Table IV-2.1-2 Critical Constant

	Critical temperature	Critical pressure	Critical specific volume
Ammonia	405.4K 132.35°C	11.304×10^6Pa 113.04bar	72.46×10^{-3}m^3/kmol 4.255×10^{-3}m^3/kg
Water	647.30K 374.15°C	22.12×10^6Pa 221.2bar	57.11×10^{-3}m^3/kmol 3.170×10^{-3}m^3/kg

Table IV-2.1-3 Reference State Specified by `KSTAN`

KSTAN	Standard state and value of enthalpy and entropy
0	comforms to reference[1] Ammonia T_0 =322.52K, p_0 =20.0bar, T_B =100K : h^l_{oR} =h^l_o/(RT_B)=4.878573kJ/kmol : h^v_{oR} =h^v_o/(RT_B)=26.468879kJ/kmol : s^l_{oR} =s^l_o/R=1.644773kJ/(kmol·K) : s^v_{oR} =s^v_o/R=8.339026kJ/(kmol·K) Water T_0 =507.05K, p_0 =30.0bar, T_B =100K : h^l_{oR} =h^l_o/(RT_B)=21.821141kJ/kmol : h^v_{oR} =h^v_o/(RT_B)=60.965058kJ/kmol : s^l_{oR} =s^l_o/R=5.733498kJ/(kmol·K) : s^v_{oR} =s^v_o/R=13.453430kJ/(kmol·K)
1	enthalpy and entropy of saturated liquid pure ammonia at 273.15K 200kJ/kg, 1kJ/(kg·K) enthalpy and entropy of saturated liquid pure water at 273.15K 200kJ/kg, 1kJ/(kg·K)
others	the same with when KSTAN=0

2.1.4 Formula

A correction to [1] has been made as below.

11th term of r.h.s. of eq.(7) : $C_2(P_r/T_r^3 - 4P_{r,0}/T_r^3 + 3P_{r,0}T_r/T_{r,0}^4)$
$\rightarrow C_2(P_r/T_r^3 - 4P_{r,0}/T_{r,0}^3 + 3P_{r,0}T_r/T_{r,0}^4)$

2.1.5 Valid Range

0.2[bar]<p<110[bar]
230[K]<T<600[K]

2.1.6 Example of User's PROGRAM UNIT

Sample Program 1

example1.for :

```
c     ------------------------------------------------
c       This program calculates temperature at bubble
c       point (p=8[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,V,H,S
      INTEGER I,J
C
c     ---------------------------------------------
c       T=[deg],p=[bar],quantity=[kg]
c       standard state=(273.15[K],saturated liquid)
c     ---------------------------------------------
      CALL KPAMES(1,1)
      CALL STNKAS(1,1)
C
c     ----------------------------------------
c       Bubble point pressure using
c       subtb.
c     ----------------------------------------
      P=8.0
      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      170.330100
c      1.000000E-01      143.563200
c      2.000000E-01      118.597400
c      3.000000E-01       95.639790
c      4.000000E-01       74.913720
c      5.000000E-01       57.048260
c      6.000000E-01       42.734430
c      7.000000E-01       32.359450
c      8.000000E-01       25.701210
c      9.000000E-01       21.752430
c          1.000000       18.764890
```

Sample Program 2

example2.for :

```
c     ------------------------------------------
c       This program calculates the properties
c       in saturated state at p=1.0[bar],T=150[K]
c     ------------------------------------------
      REAL T,P,X,Y,VL,VV,HL,HV,SL,SV
      INTEGER J
C
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     ------------------------------------------
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
         STOP
      ENDIF
      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
      STOP
      END
C
c     ---------------------------------------------------------------------
c          Results
c     ---------------------------------------------------------------------
c    X[kmol NH3/kmol]=   6.188429E-01   y[kmol NH3/kmol]=   9.988968E-01
c   vL[m^3/kmol]     =   2.220031E-02  vV[m^3/kmol]     =       4.716768
c   hL[MJ/kmol]      =      -1.828154  hV[MJ/kmol]      =      22.576830
c   sL[MJ/(kmol K)]  =       4.394936  sV[MJ/(kmol K)]  =      81.492060
```

2.1.7 Sample Output of Single Shot Program

```
=========================================================================
|   Single Shot Program for Ammonia-Water Mixture,                      |
|   an Application Program by M-PROPATH Ver.9.1                         |
|   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-SS.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.9.1                        |
|   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.9.1                        |
|   Thermophysical Properties of Ammonia-Water Mixtures                |
|----------------------------------------------------------------------|
|  ## First Menu ##                                                    |
| No.                      Current                                     |
| 1 --> Go to Second Menu                                              |
| 2 --> Read Help                                                      |
| 3 --> Set Logfile       [ON] AWMIX.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         [ kg ]
 3 --> Standard Values of h and s  [1] Ibrahim & Klein
 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.
1

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

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

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

=============================================
 No.   Standard States and Values of h and s
 1 --> As defined in:
       O.M.Ibrahim and S.A.Klein, Thermodynamic
       Properties  of  Ammonia-Water  Mixtures,
       ASHRAE Transactions: Symposia, vol.99,
       1993, pp.1495
 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.
2
```

```
=====================================================
 No.                                current
=====================================================
 1 --> Pressure and Temperature    [ Pa, K]
 2 --> Amount of Substance         [kmol]
 3 --> Standard Values of h and s  [2] IIR
 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  =    .48594630[kg/kg]
 Relative Molecular Mass of Mixture =      17.52278000[kg/kmol]
 Relative Molecular Mass of Ammonia =      17.03026000[kg/kmol]
 Relative Molecular Mass of Water   =      18.01530000[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  =    .51405370[kmol/kmol]
 Relative Molecular Mass of Mixture =      17.50894000[kg/kmol]
 Relative Molecular Mass of Ammonia =      17.03026000[kg/kmol]
 Relative Molecular Mass of Water   =      18.01530000[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     18.01530000  [kg/kmol]
Gas Constants                488.18980000    461.49660000  [J/(kg*K)]
Critical Temperature         405.65000000    647.13000000  [K]
                             132.50000000    373.98000000  [C]
Critical Pressure            112.78000000    220.55000000  [bar]
```

```
Critical Volume             .72470000E-01   .55950000E-01  [m**3/kmol]
                            .42553670E-02   .31056930E-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[Pa]          (P=0 : Second Menu)
100000.0
Input T[K]
250.0
Input Z[kmol/kmol]
0.5
T  =     250.00000000[K]          P  =     100.00000000[kPa]
Z  =        .50000000[kmol/kmol]  H  =   -2604.64600000[kJ/kmol]
S  =       7.09724800[kJ/(kmol*K)]V  =    .20689990E-01[m**3/kmol]
Liquid Region

Input P[Pa]          (P=0 : Second Menu)
100000.0
Input T[K]
300.0
Input Z[kmol/kmol]
0.5
T  =     300.00000000[K]          P  =     100.00000000[kPa]
Z  =        .50000000[kmol/kmol]  H  =    8604.31400000[kJ/kmol]
S  =      47.05576000[kJ/(kmol*K)]V  =    .64970690E+01[m**3/kmol]
X  =        .32842270[kmol/kmol]  Y  =        .98106720[kmol/kmol]
HL =    2107.11700000[kJ/kmol]    HV =   26821.11000000[kJ/kmol]
SL =      23.16687000[kJ/(kmol*K)]SV =     114.03530000[kJ/(kmol*K)]
VL =    .19941250E-01[m**3/kmol]  VV =    .24657600E+02[m**3/kmol]
QUALITY =       .26289550[kmol/kmol]

Input P[Pa]          (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[Pa]          (P=0 : Second Menu)
100000.0
Input Z[kmol/kmol]
0.5
Input H[J/kmol]
-2604646.0
T  =     250.00000000[K]          P  =     100.00000000[kPa]
Z  =        .50000000[kmol/kmol]  H  =   -2604.64600000[kJ/kmol]
S  =       7.09724600[kJ/(kmol*K)]V  =    .20689990E-01[m**3/kmol]
Liquid Region

Input P[Pa]          (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[Pa]          (P=0 : Second Menu)
100000.0
Input Z[kmol/kmol]
0.5
Input S[J/(kmol*K)]
7097.248
T  =     250.00000000[K]          P  =     100.00000000[kPa]
Z  =        .50000000[kmol/kmol]  H  =   -2604.64600000[kJ/kmol]
S  =       7.09724900[kJ/(kmol*K)]V  =    .20689990E-01[m**3/kmol]
Liquid Region

Input P[Pa]          (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[Pa]          (P=0 : Second Menu)
100000.0
Input Z[kmol/kmol]
0.5
Input V[m**3/kmol]
0.02068999
T  =     256.96330000[K]          P  =     100.00000000[kPa]
Z  =        .50000000[kmol/kmol]  H  =   -2024.96600000[kJ/kmol]
S  =       9.38436200[kJ/(kmol*K)]V  =    .20689990E-01[m**3/kmol]
Liquid Region

Input P[Pa]          (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[Pa]          (P=0 : Second Menu)
100000.0
Input Z[kmol/kmol]
0.5
P  =     100.00000000[kPa]        Z  =        .50000000[kmol/kmol]
TB =     272.16450000[K]          TD =     355.92290000[K]
HB =    -790.82810000[kJ/kmol]    HD =   39835.19000000[kJ/kmol]
SB =      14.05111000[kJ/(kmol*K)]SD =     139.75980000[kJ/(kmol*K)]
VB =    .20754300E-01[m**3/kmol]  VD =    .29210500E+02[m**3/kmol]

Input P[Pa]          (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[kmol/kmol]   (Z < 0 : Second Menu)
0.5
Input T[K]
300.0
T  =     300.00000000[K]          Z  =        .50000000[kmol/kmol]
PB =     296.73480000[kPa]        PD =       6.83075500[kPa]
HB =    1411.31000000[kJ/kmol]    HD =   38011.88000000[kJ/kmol]
SB =      21.74171000[kJ/(kmol*K)]SD =     156.36270000[kJ/(kmol*K)]
VB =    .21098430E-01[m**3/kmol]  VD =    .36442130E+03[m**3/kmol]

Input Z[kmol/kmol]   (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[Pa]          (P=0 : Second Menu)
100000.0
Input T[K]
300.0
T  =     300.00000000[K]          P  =     100.00000000[kPa]
X  =        .32842270[kmol/kmol]  Y  =        .98106720[kmol/kmol]
HL =    2107.11700000[kJ/kmol]    HV =   26821.11000000[kJ/kmol]
SL =      23.16687000[kJ/(kmol*K)]SV =     114.03530000[kJ/(kmol*K)]
VL =    .19941250E-01[m**3/kmol]  VV =    .24657600E+02[m**3/kmol]

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

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

References

[1] O.M.Ibrahim and S.A.Klein, Thermodynamic properties of ammonia-water mixtures, ASHRAE Transactions:Symposia, CH-93-21-2, 1993